PB 206 144

CATALOG OF PESTICIDE NMR SPECTRA

A. L. Alford, et al

Environmental Protection Agency
Athens, Georgia

April 1971

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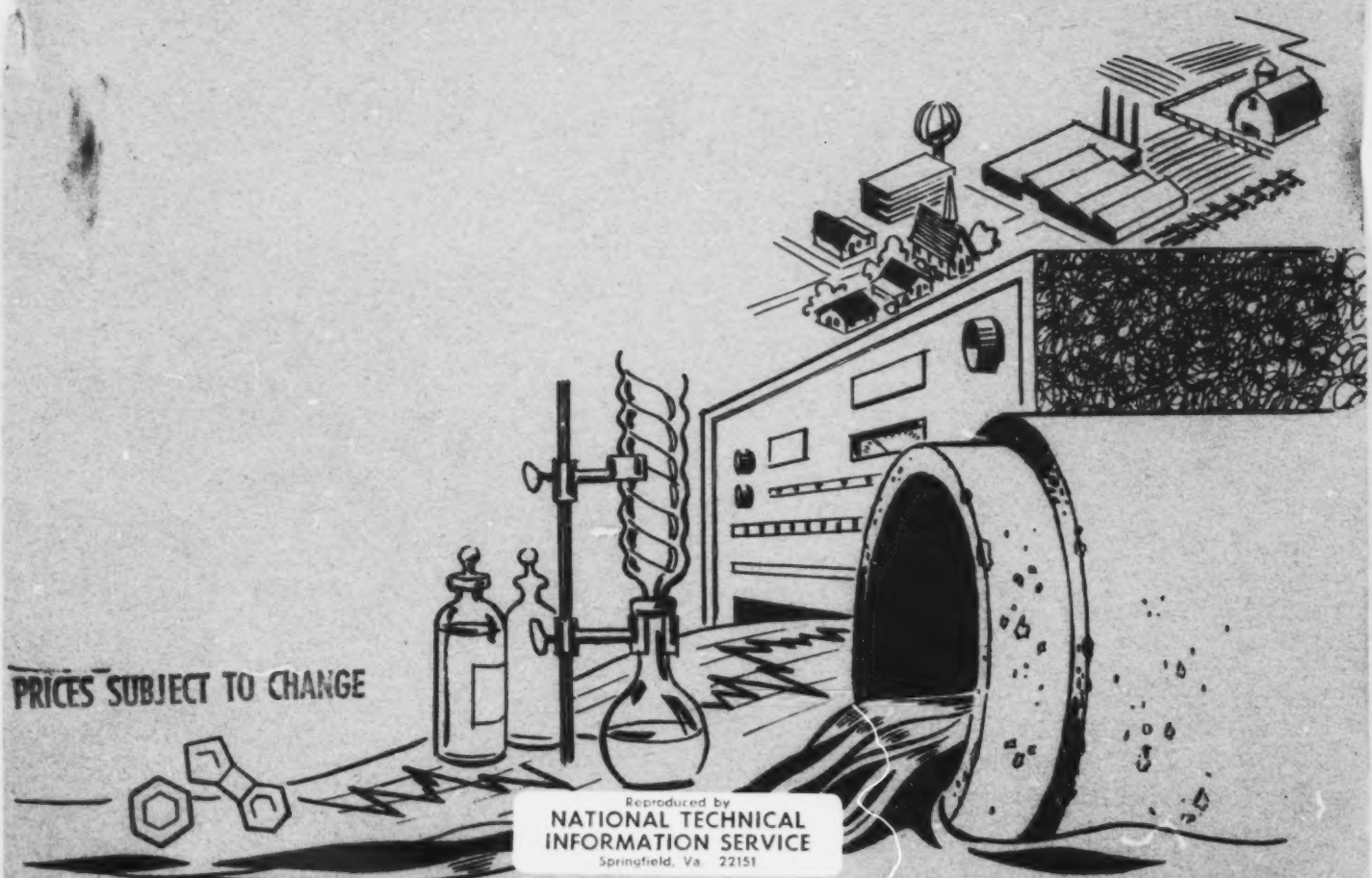
Catalog of Pesticide

NMR Spectra



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16. Abstract

Nuclear magnetic resonance spectra have been recorded, interpreted, and published for organophosphorus pesticides, DDT and related compounds, and carbamate pesticides and some of their degradation products. A Varian HA-100 NMR spectrometer with a variable-temperature probe and a homonuclear spin decoupler was used to record the spectra of 114 compounds. Chemical shifts and coupling constants are shown for each spectrum. The chemical name and source of each pesticide are listed. (Holoman-Battelle)

17a. Descriptors

*Organophosphorus pesticides, *DDT, *Carbamate pesticides, *Nuclear magnetic resonance, Pesticides, Spectroscopy, Pollutant identification, Diazinon,

17b. Identifiers

*Chemical shifts, *Coupling constants, Spin decoupling, Metabolites, NMR spectra, Malathion, Malaoxon, Cygon, Dimethoxon, Meta-Systox-R, Dibrom, Neguvon, DDVP, Ciodrin, Azodrin, Bidrin, Phosdrin, Phosphamidon, Methyl Trithion, Guthion, Guthion oxygen analog, Imidan, Tiguvon, Abate, Ronnel, Gardona, Methyl parathion, Sumithion, Dicapthon, Ruelene, Zytron, Thimet, Di-Syston,
(Continued on next page)

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Abstractor Verna L. Holoman | Institution Analytical Quality Control Lab., EPA, Cincinnati

CATALOG OF PESTICIDE

NMR SPECTRA

by

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April 1971

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ABSTRACT

This catalog contains the 100-MHz NMR spectra of 114 organophosphorus, DDT, and carbamate pesticides and a brief discussion of their most important features. Chemical shifts and coupling constants are shown on each spectrum.

CONTENTS

Section		Page
I	Introduction	1
II	Experimental	3
III	Discussion	
	A. The Organophosphorus Pesticides	5
	B. DDT and Related Compounds	61
	C. The Carbamate Pesticides	93
IV	Index to Spectra	137
V	Acknowledgments	149
VI	References	151
VII	List of Publications Resulting from this Work	153
VIII	Appendix: Chemical Names and Sources of the Pesticides	155

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SECTION I

INTRODUCTION

Pesticides are important sources of water contamination. Individual pesticides or their degradation products must often be identified if the water quality is to be protected and improved. Nuclear magnetic resonance (NMR) spectroscopy provides unique structural information (1) that cannot be obtained from infrared spectroscopy, mass spectrometry, and gas chromatography (the primary instrumental methods currently used to identify water contaminants).

Interpretation of NMR spectra is enhanced when spectra of known similar compounds are available for comparison. Since few pesticides have been included in NMR spectral catalogs, we recorded and interpreted spectra of three important classes of pesticides and some of their degradation products. Spectral interpretations were discussed in previous publications (2-5), but only a few spectra were included.

This catalog contains spectra of 114 compounds arranged according to molecular structures:

1. Organophosphorus pesticides
   a. Phosphomethoxy [$(CH_3O)_2$-P]
   b. Phosphoethoxy [$(C_2H_5O)_2$-P]
   c. Miscellaneous
2. DDT and related compounds -- pesticides and several known or proposed metabolites with the substitute diphenyl methane skeleton.
3. Carbamate pesticides.

Chemical names and sources of the compounds are listed in the Appendix in the order they appear in this publication. Section IV is an alphabetical index of the common names and trade names of all compounds in this catalog.

SECTION II

EXPERIMENTAL

The 100-MHz spectra were recorded with a Varian HA-100 NMR spectrometer equipped with a variable-temperature probe and a homonuclear spin decoupler. Solutions (300 mg/ml) were prepared in deuterochloroform, except when other solvents or less concentrated solutions had to be used, or when changing solvent or concentration produced a desirable chemical shift. Each spectrum shows chemical shifts (τ values with reference to the internal standard, tetramethylsilane). Sweep widths of 1000 Hz or 500 Hz were used, but portions of some spectra were expanded for more detailed analysis. In some cases homonuclear spin decoupling, integration, protonation with trifluoroacetic acid, D_2O exchange, temperature, solvent and concentration variations, and supplemental 60-MHz spectra were needed for spectral interpretation.

SECTION III

DISCUSSION

THE ORGANOPHOSPHORUS PESTICIDES

Signal splittings due to coupling of phosphorus with hydrogen complicate these spectra. Coupling constants, inversely proportional to the P-H distance, vary from 0.5 to 18 Hz. The aromatic proton signals of ronnel, dicapthon, Ruelene, Zytron, methyl parathion, ethyl parathion and paraoxon, have a small splitting due to P-H coupling through four and/or five bonds. The phosphoethoxy methyl signals (τ 8.59-8.67, J = 0.5-1.2 Hz) also show P-H coupling through four bonds.

Each spectrum of the phosphomethoxy compounds exhibits a doublet (J = 11-16 Hz, τ 6.1-6.3) due to the CH_3O-P protons coupled through oxygen to phosphorus. In malathion, malaoxon, Dibrom, and Neguvon, each doublet exhibits a smaller splitting (<2Hz). Two methoxyl groups are attached to the phosphorus atom and an asymmetric carbon atom is present; therefore, this splitting is actually a chemical shift difference due to a small magnetic non-equivalence of the methoxyl groups. Similarly, methylene groups of several phosphoethoxy compounds (Thimet, Di-Syston, Trithion and ethion) produce 16, rather than the expected eight, peaks. Each non-equivalent methylene group is coupled with methyl protons to produce a quartet that is further split by phosphorus. The signals of the phospho-ethoxy methylene protons appear at τ5.65-5.91 with P-H coupling of 8-10 Hz.

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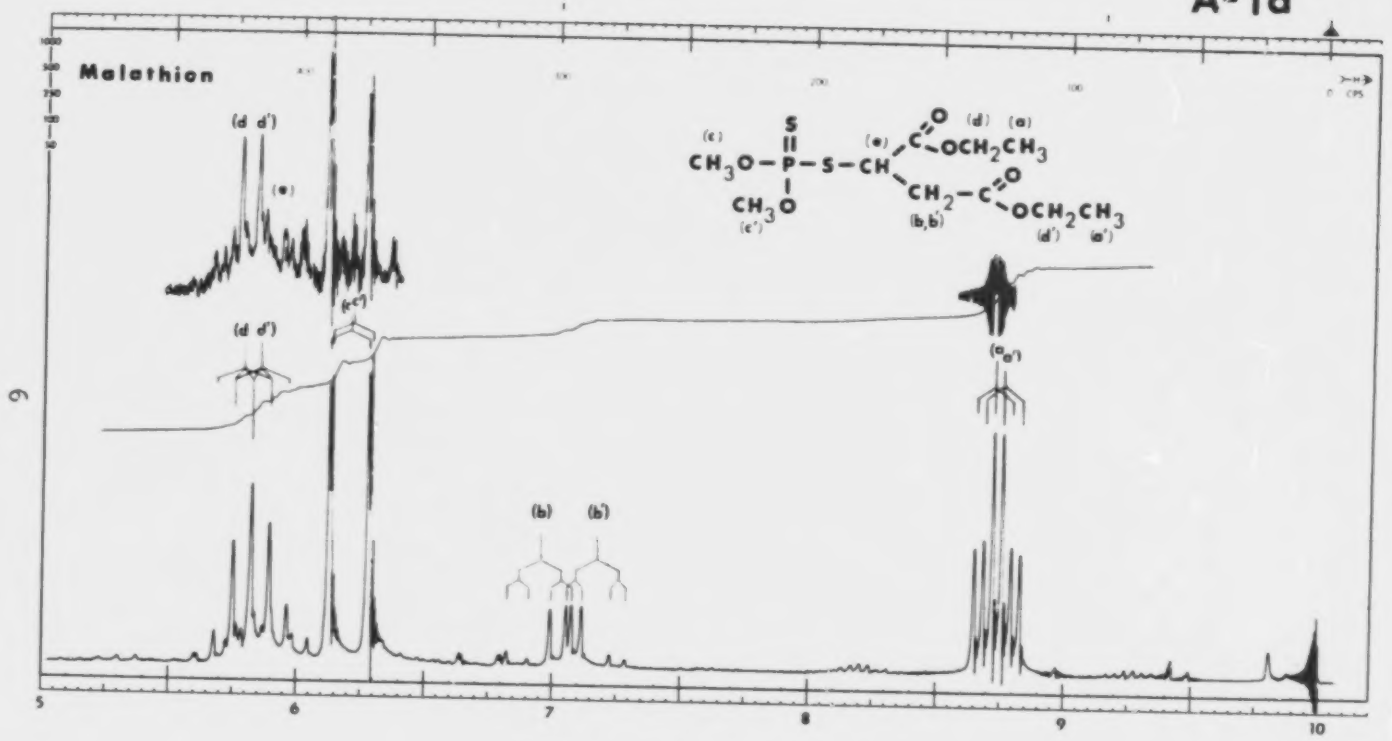
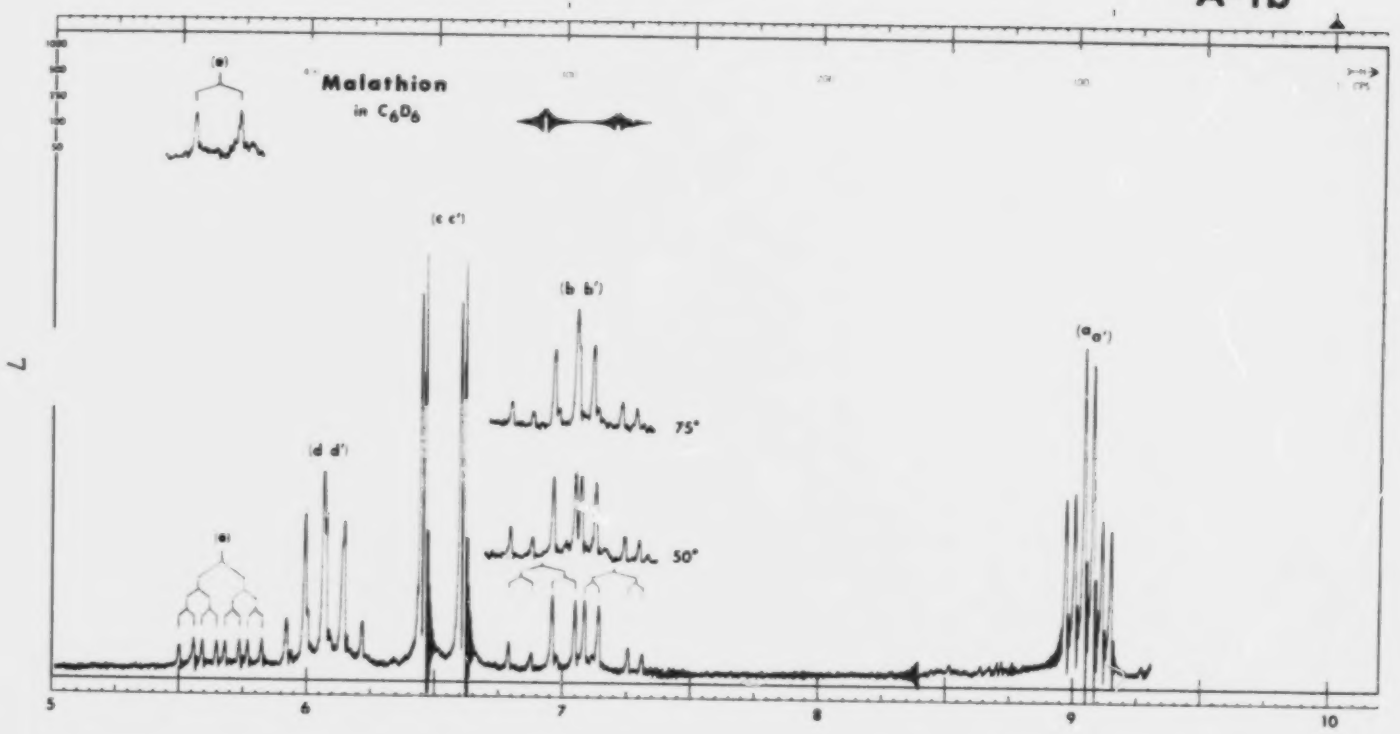
A-1a



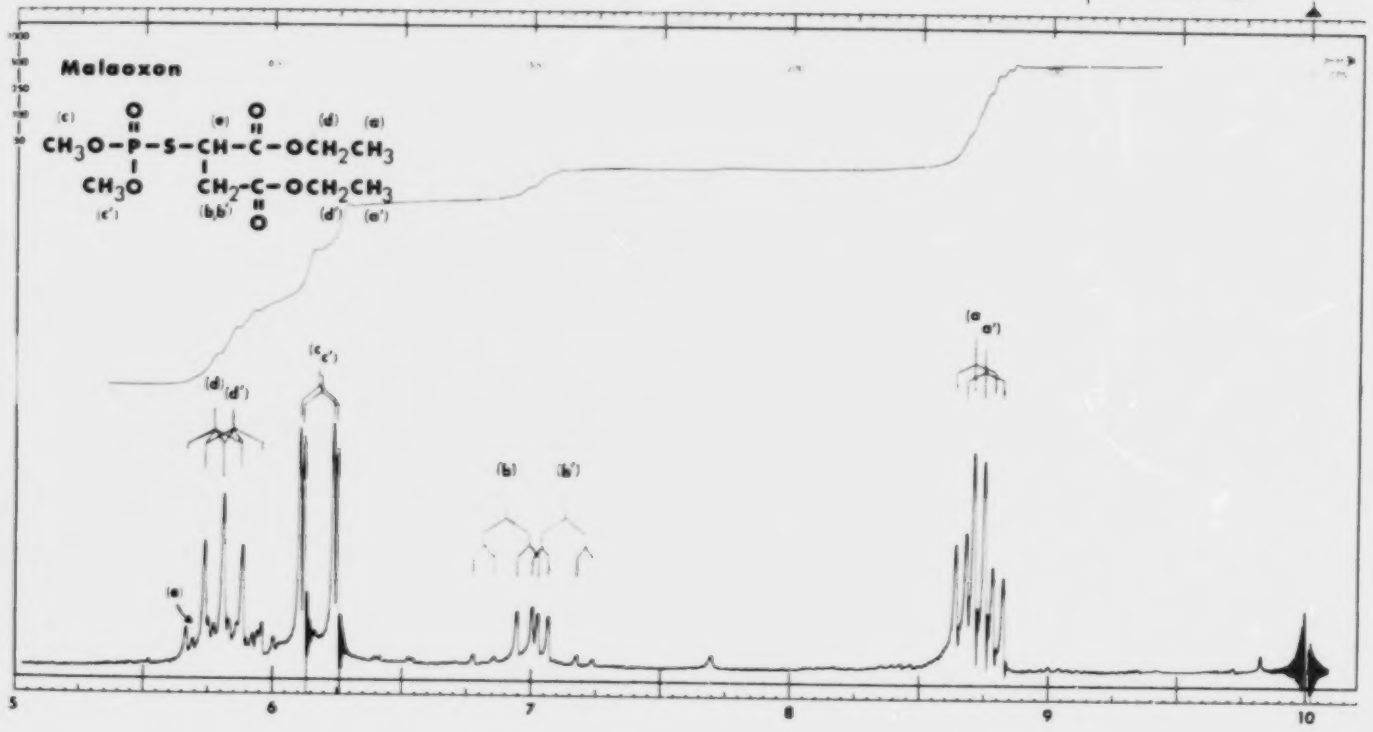
	T	J
a	8.71	7
a'	8.75	7
b	^{a}6.93	< 9 (vic.) < 17 (gem.)
b'	^{a}7.19	< 6.0 (vic.)
c	6.19	15.5 (P-H)
c'	6.20	15.5 (P-H)
d	5.78	7
d'	5.85	7
e	5.9	

A-1b



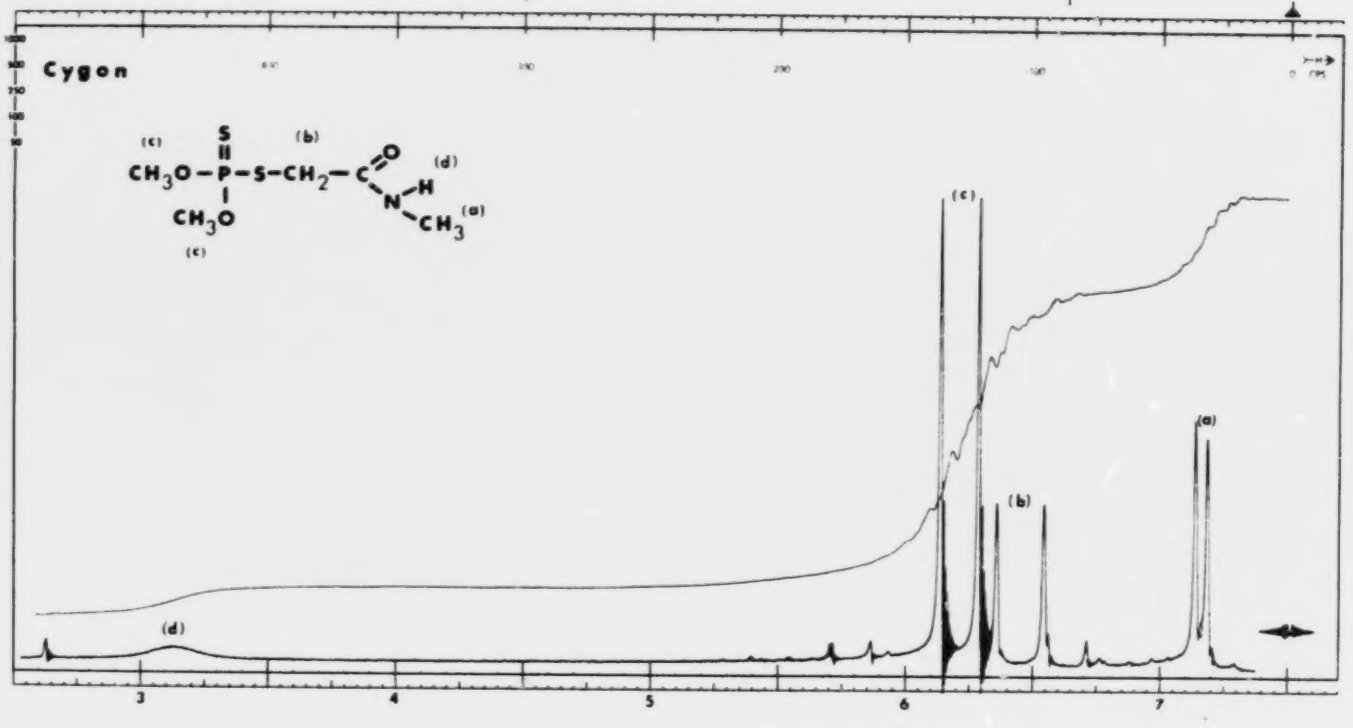
	τ	J
a	9.04	7
a'	9.08	7
b	6.90	9 (vic.)
		17 (gem.)
b'	7.22	6 (vic.)
c	6.52	15.5(P-H)
c'	6.54	15.5(P-H)
d	6.03	7
d'	6.10	7
e	5.67	17.5(P-H) 9 ($H-H_b$) 6 ($H-H_b$)

A-2



	T	J
a	8.71	7
a'	8.75	7
b	*6.88	8 (vic.)
		17 (gem.)
b'	*7.15	6 (vic.)
c	6.17	13
c'	6.18	13
d	5.78	7
d'	5.85	7
e	5.9	

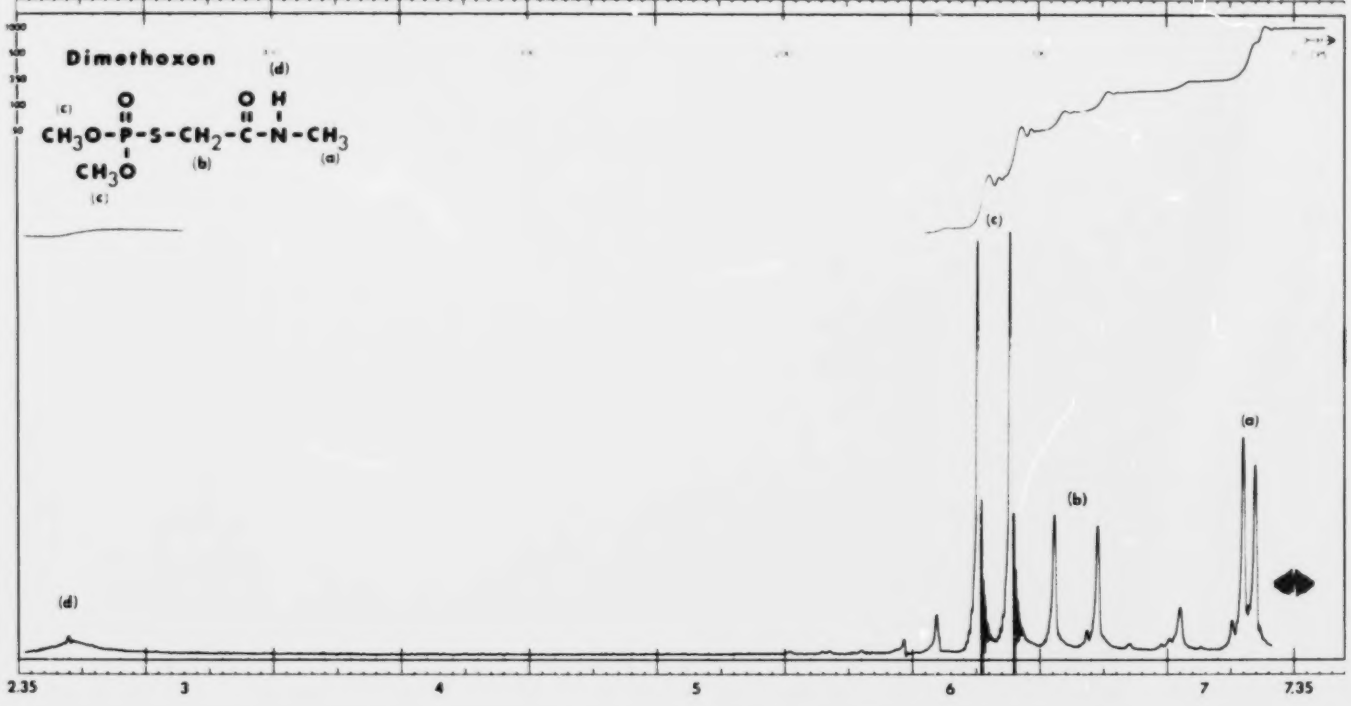
A-3



	T	J
a	7.15	4.5
b	6.44	18
c	6.20	15
d	3.13	

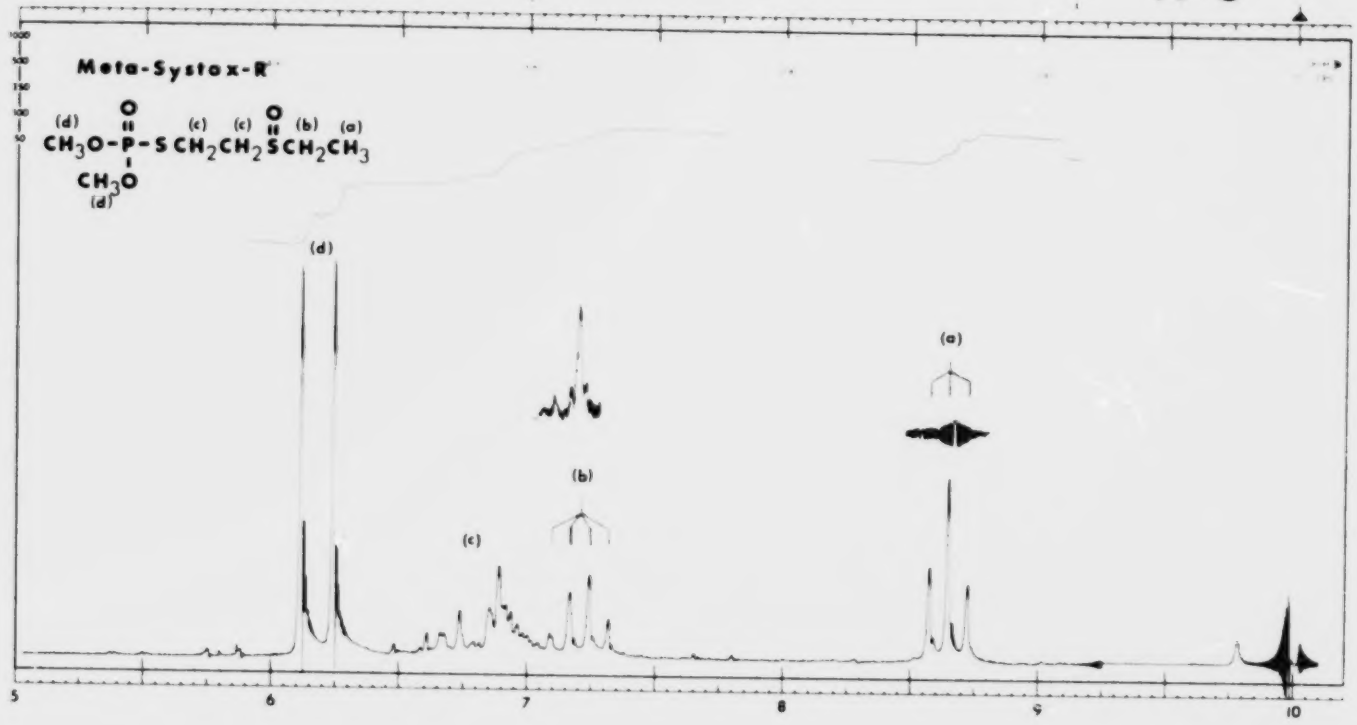
A-4

Dimethoxon



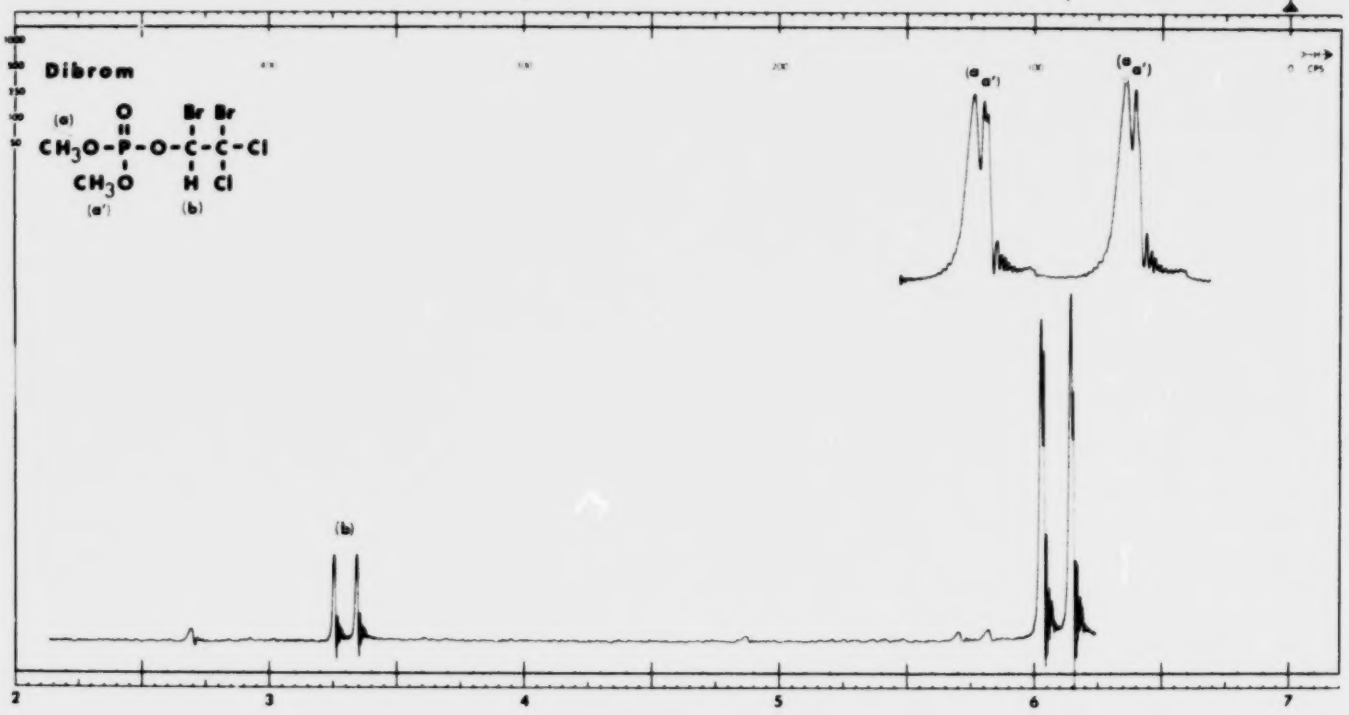
	T	J
a	7.17	5
b	6.49	17
c	6.17	12.5
d	2.55	

A-5

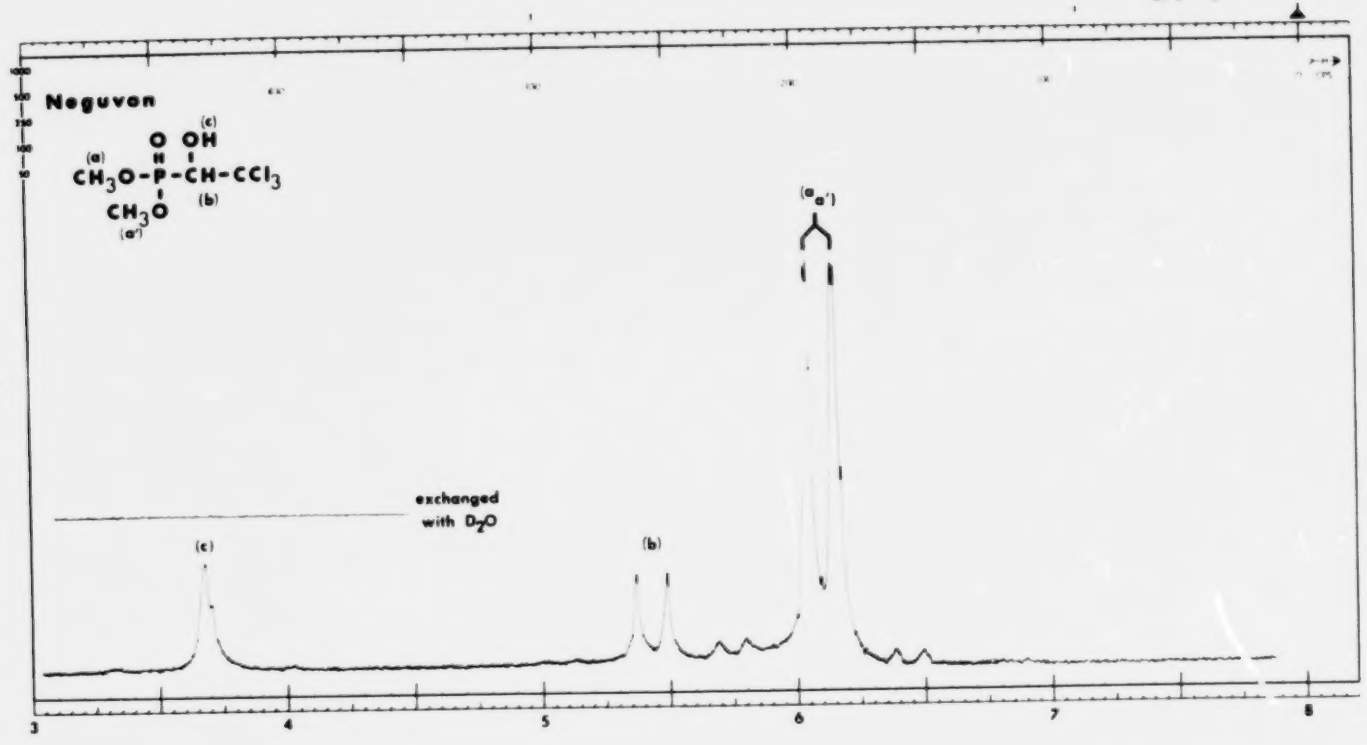


	T	J
a	8.65	7
b	7.21	7
c	6.8	
d	6.18	13

A-6

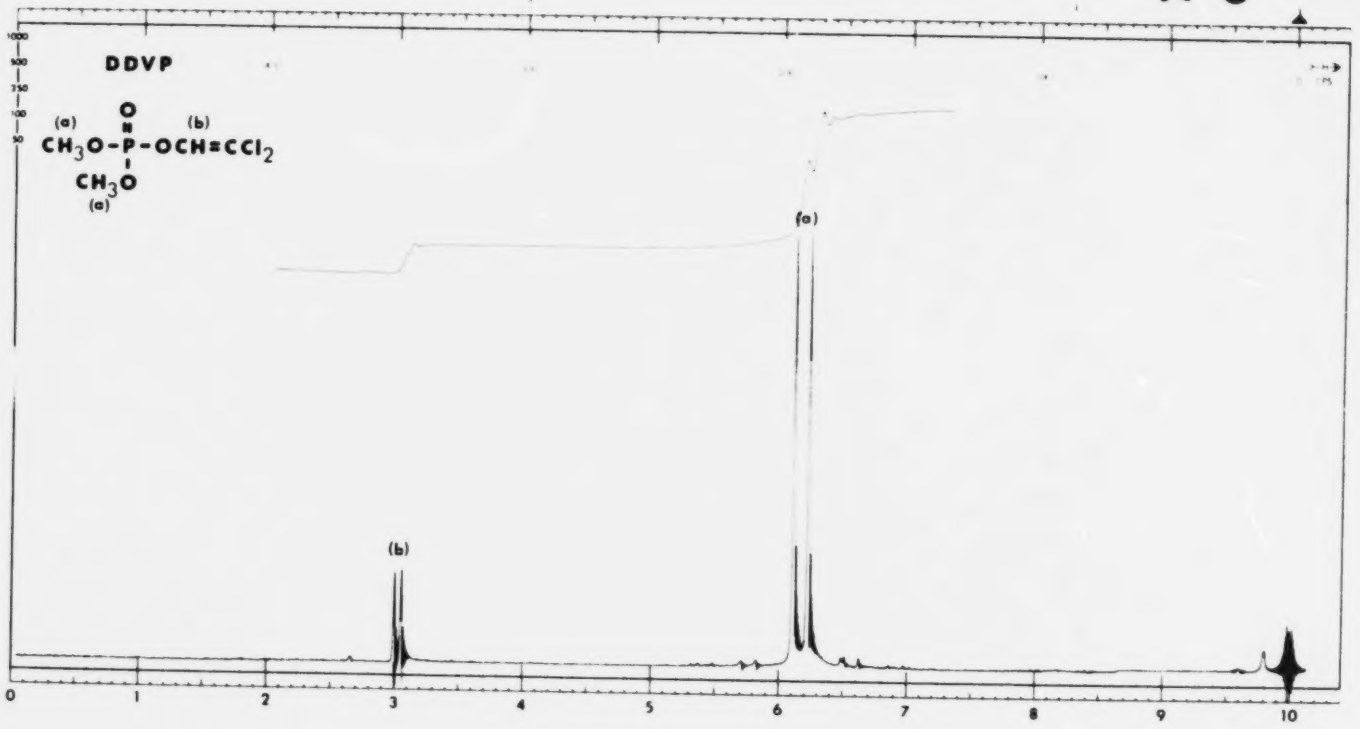


	T	J
a	6.08	12 (P-H)
a'	6.09	12 (P-H) / 0.3 (H-H)
b	3.30	9



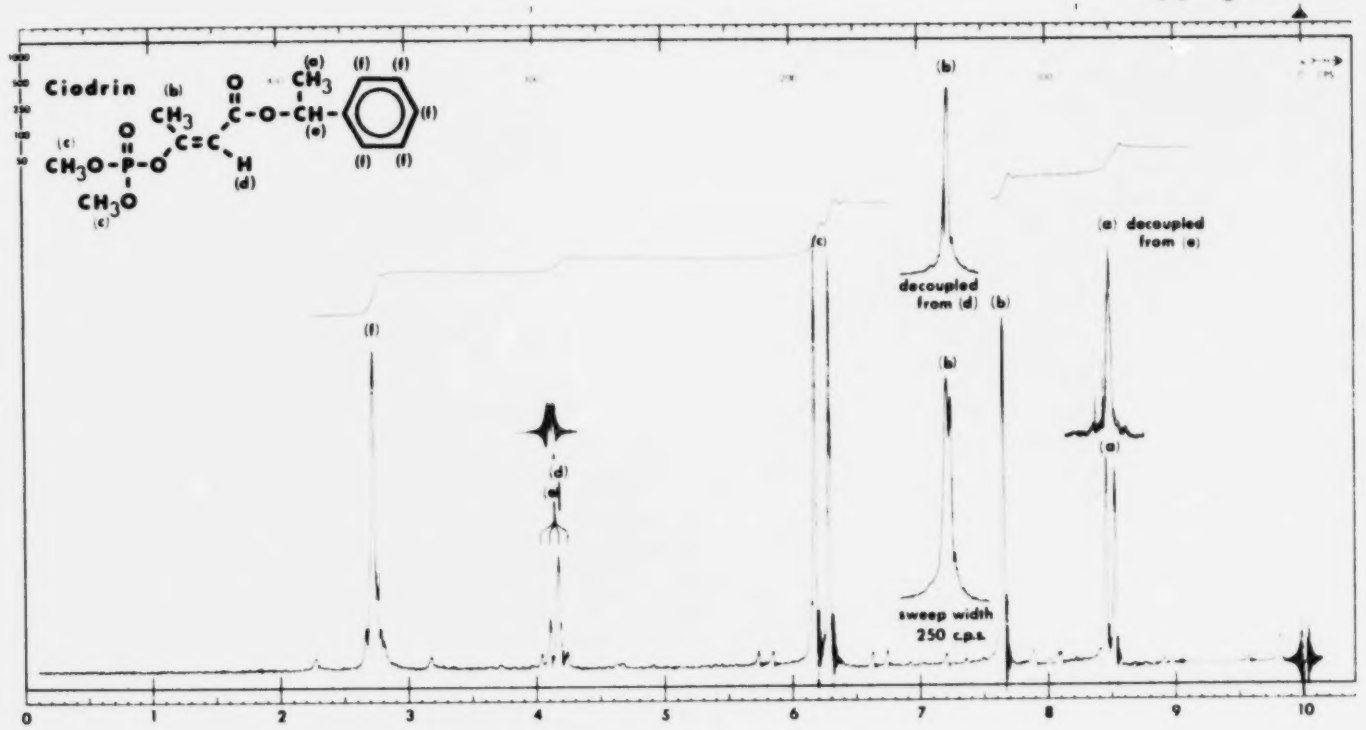
	T	J
a	6.09	11 (P-H)
a'	6.10	11 (P-H)
b	5.43	12 (P-H)
c	3.69	

A-8

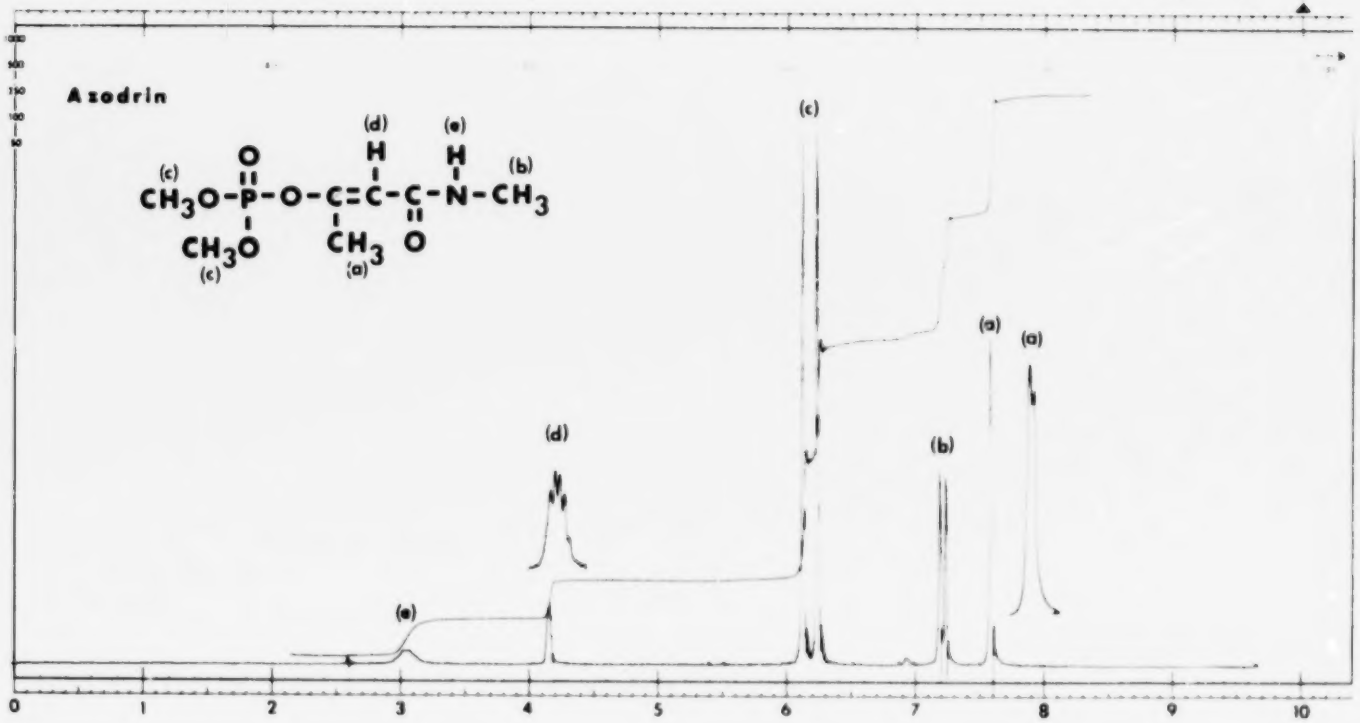


	T	J
a	6.14	11
b	3.00	5.5

A-9

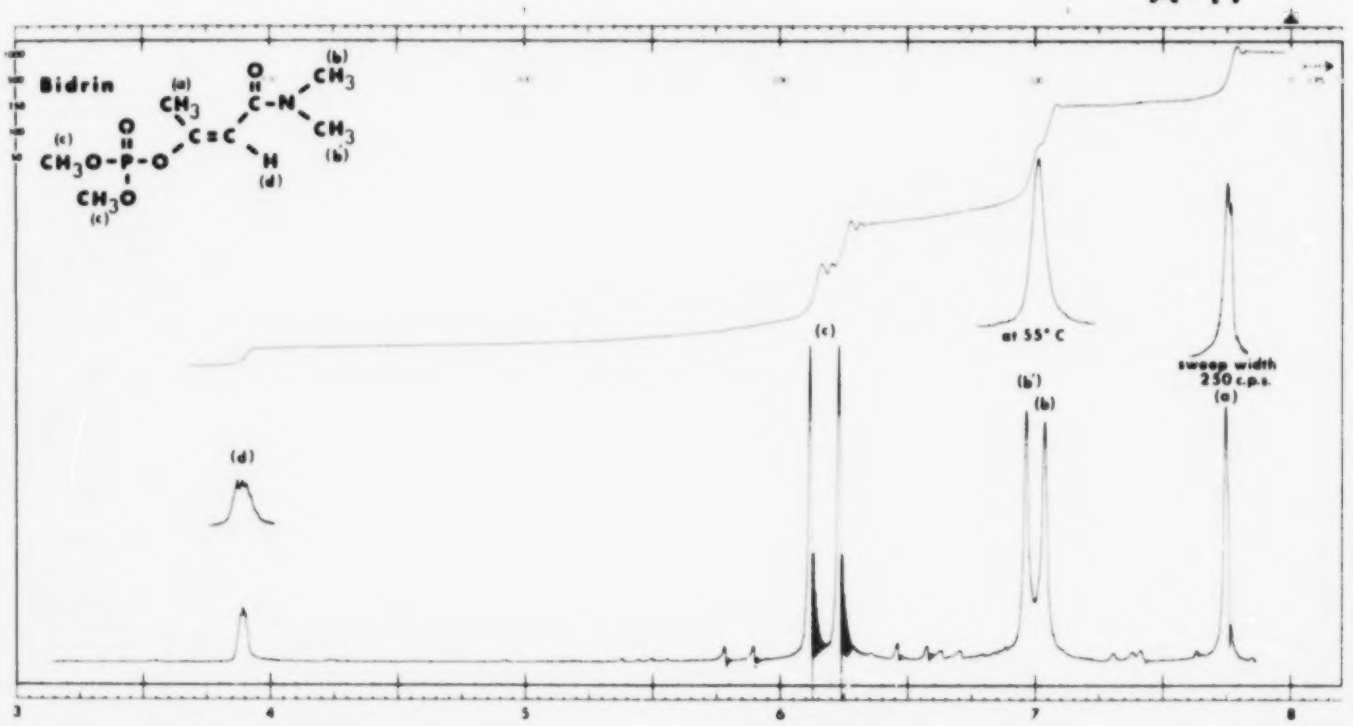


	τ	J
a	8.48	7
b	7.63	0.8
c	6.20	11 (P-H)
d	4.14	
e	4.10	7
f	2.70	



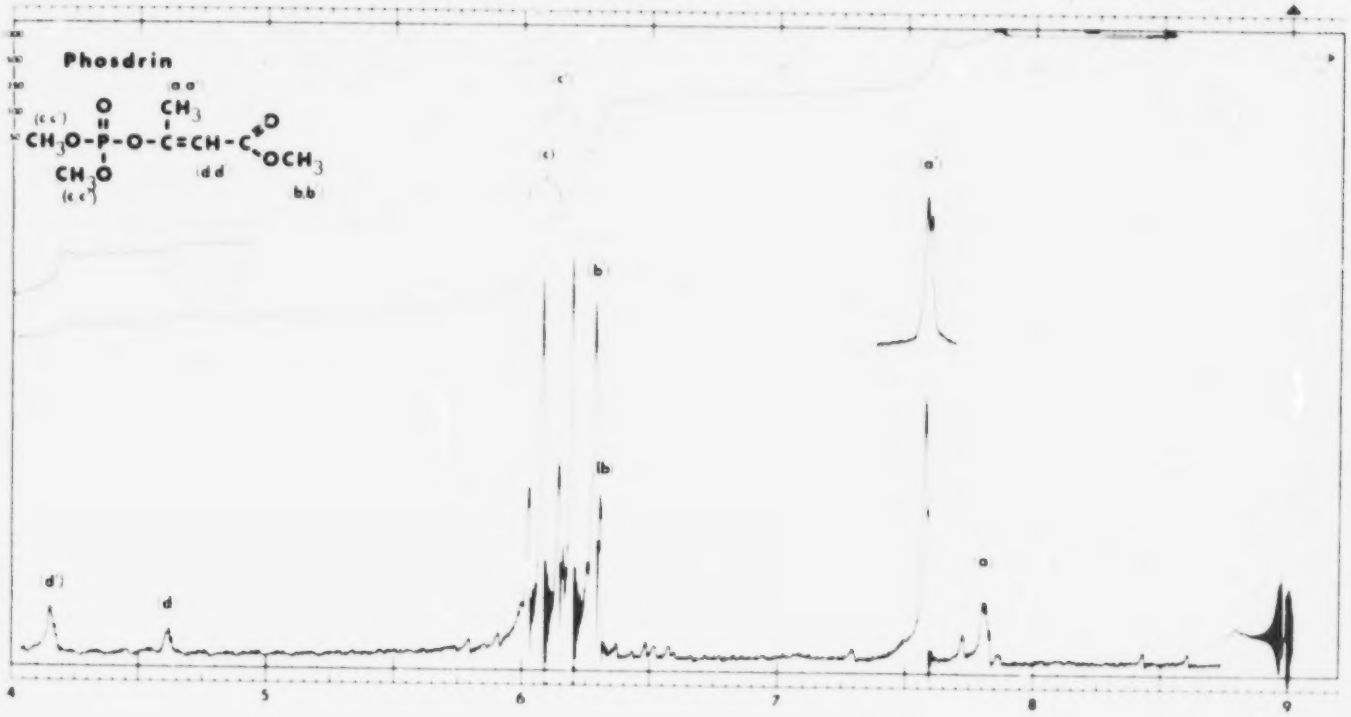
	T	J
a	7.58	0.9
b	7.21	5
c	6.16	11 (P-H)
d	4.21	0.9
e	3.0	

A-11

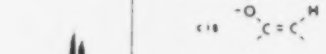


	τ	J
a	7.74	0.5
b	7.03	
b'	6.96	
c	6.17	11
d	3.89	

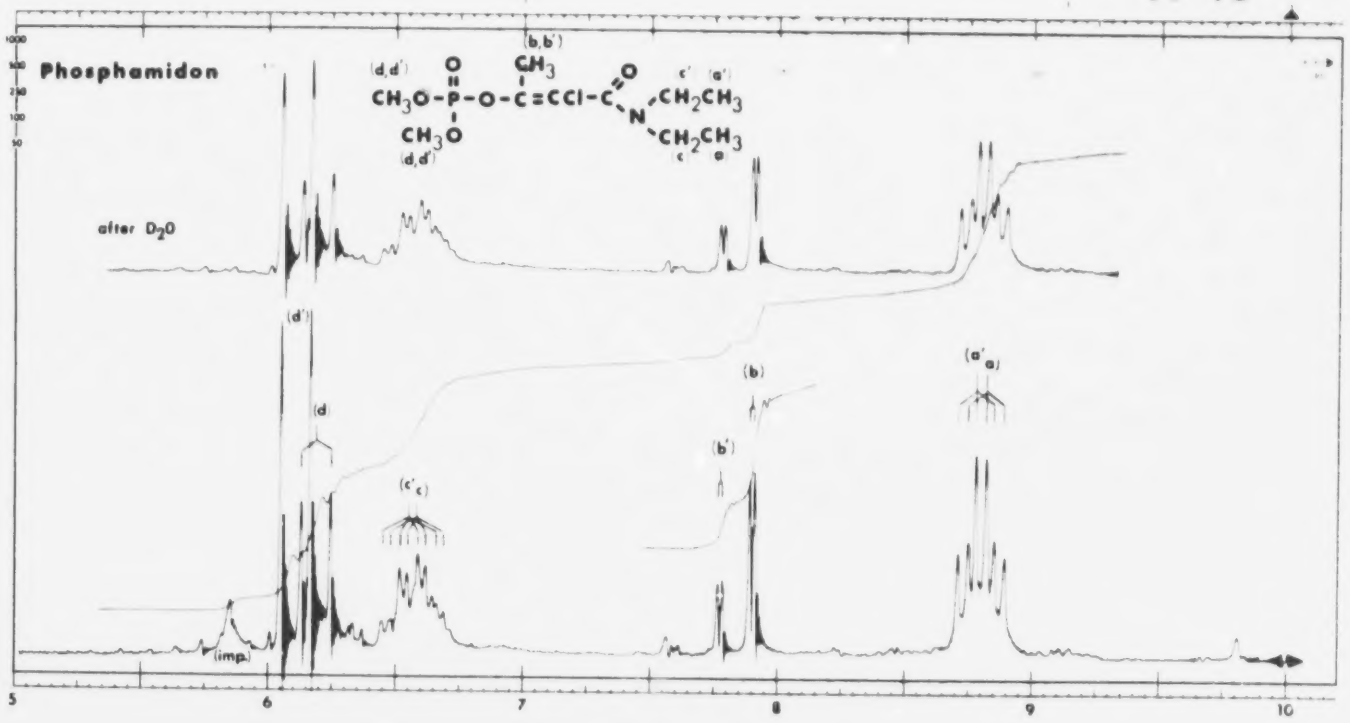
A-12



		T	J
a	trans	7.81	1.0
a'	cis	7.58	0.7
b	trans	6.31	
b'	cis	6.29	
c'	cis	6.14	11.5
c	trans	6.09	11.5
d	trans	4.62	
d'	cis	4.15	

cis 

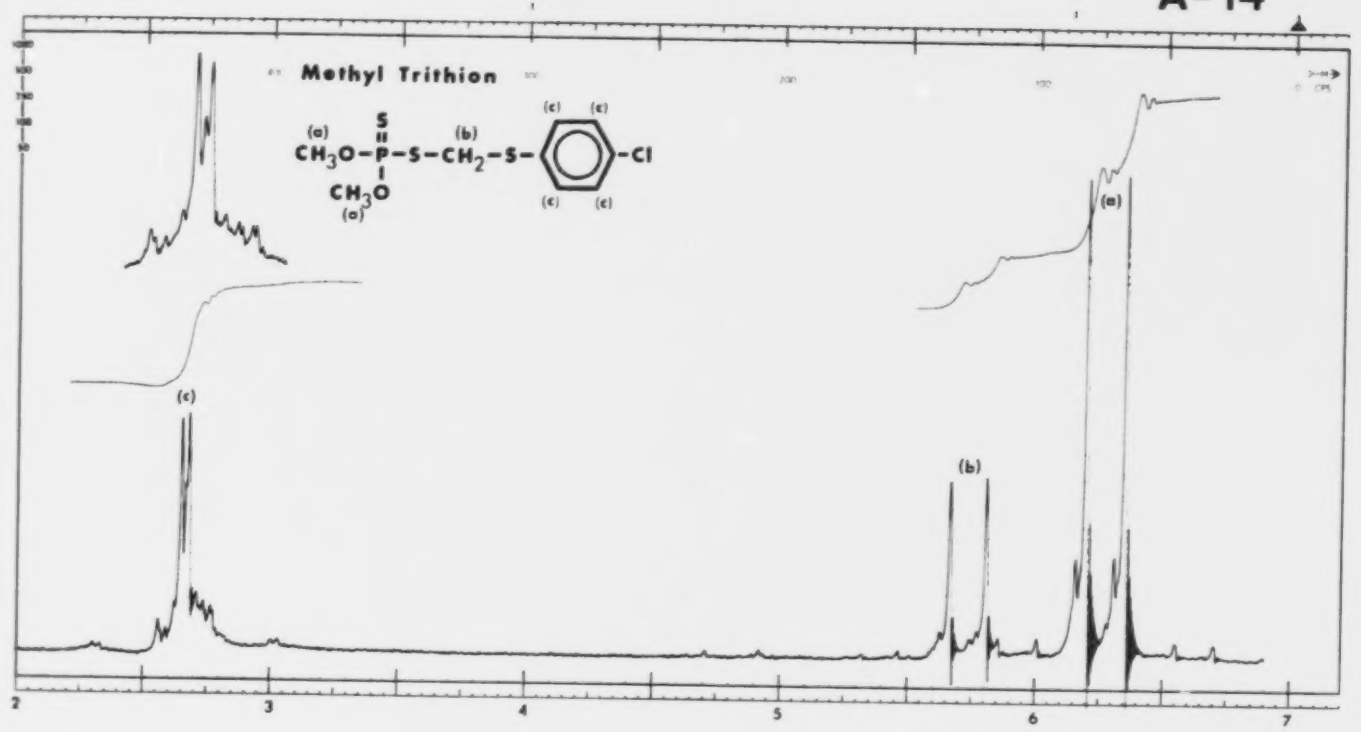
trans



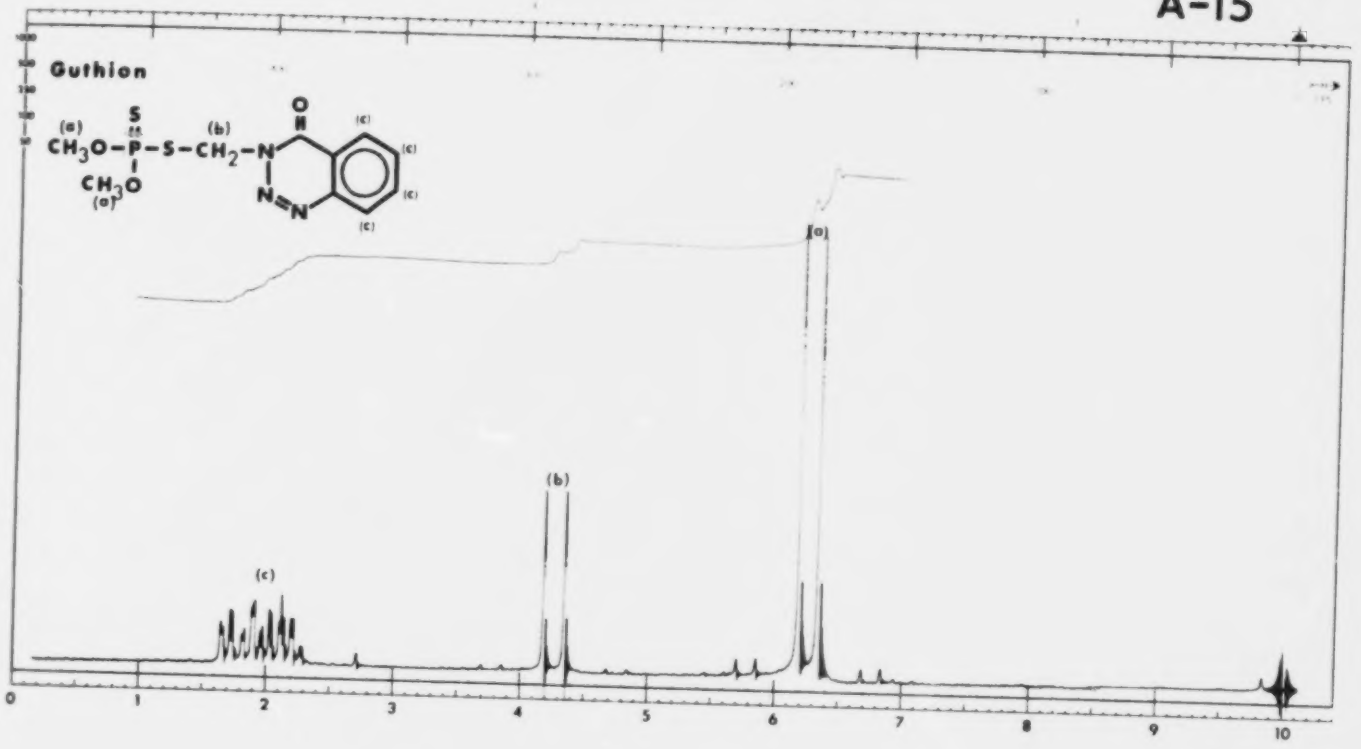
	T	J
a	8.83	7
a'	8.79	7
b trans	7.90	1.6
b' cis	7.78	1.6
c	6.59	7
c'	6.56	7
d cis	6.20	12
d' trans	6.12	12

trans

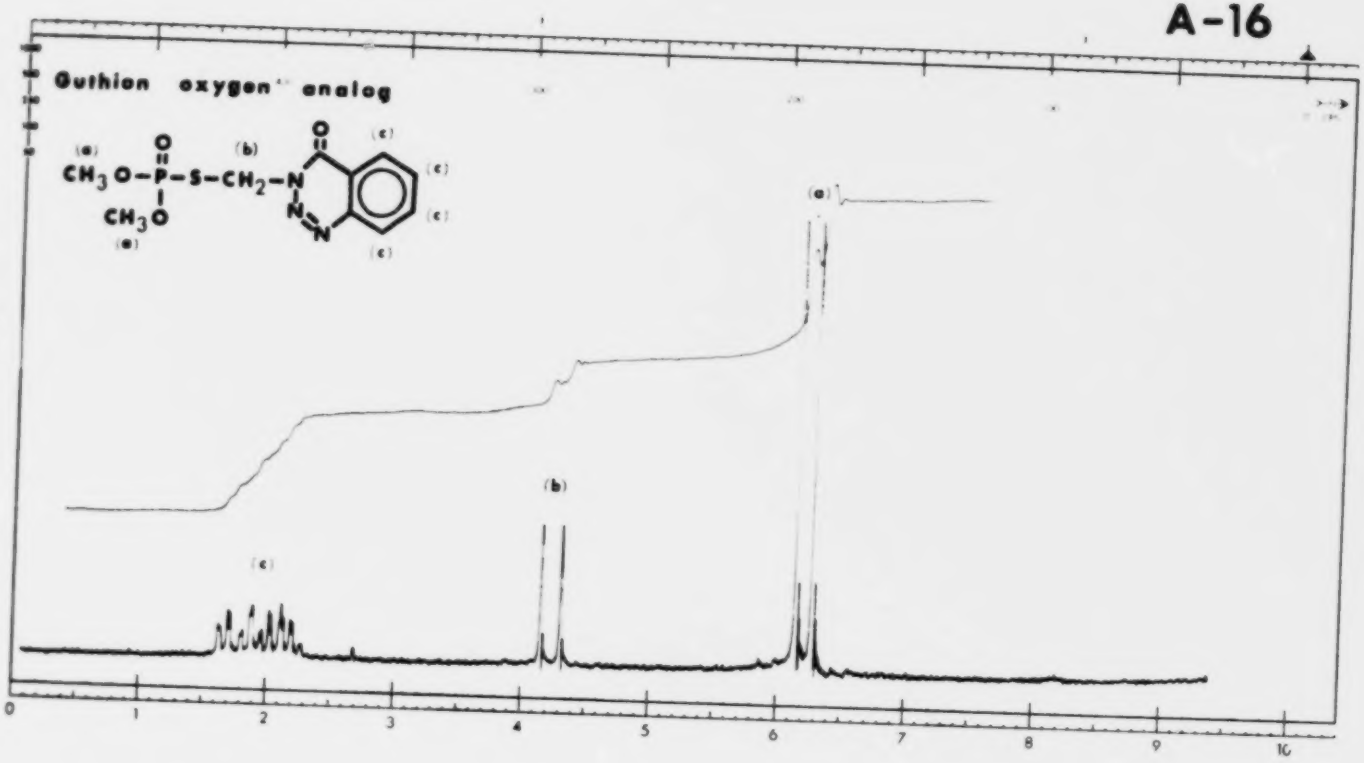
cis



	T	J
a	6.28	15
b	5.74	14
c	2.67	



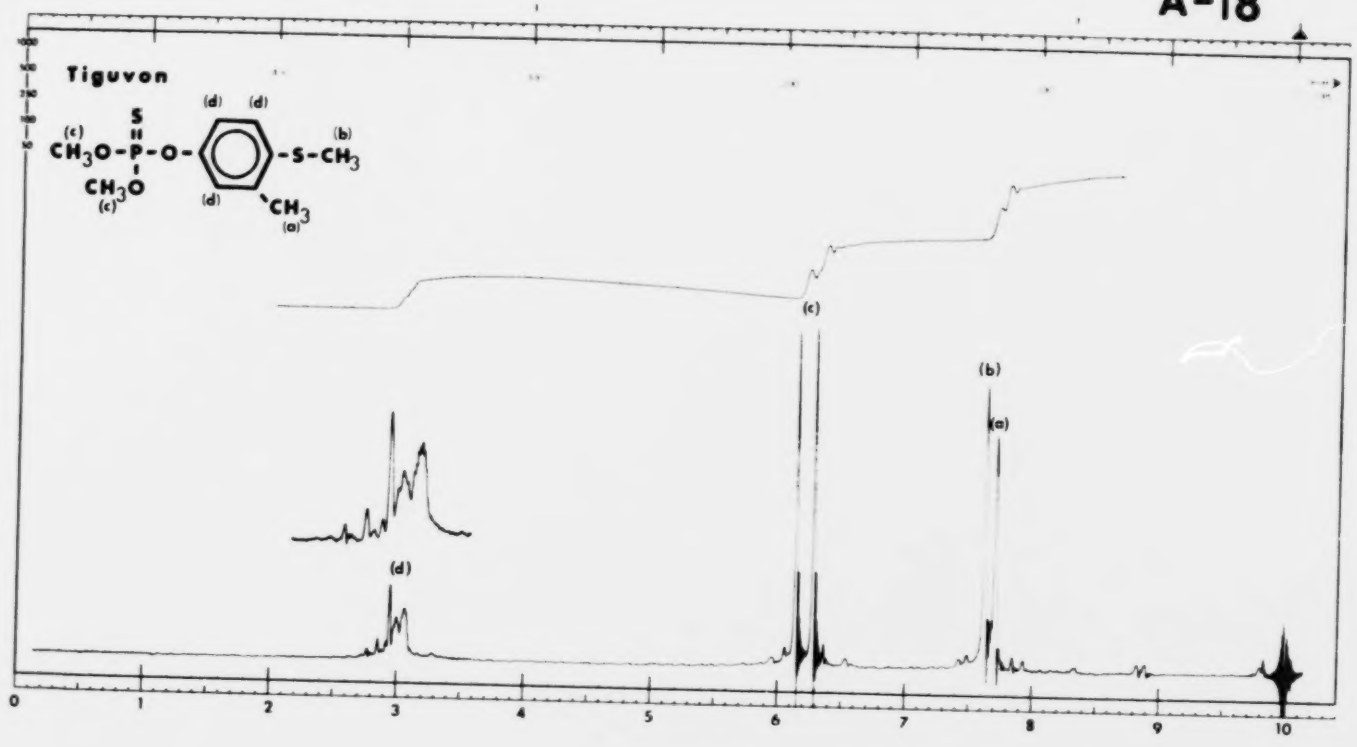
	T	J
a	6.24	15
b	4.23	16
c	1.9	



	T	J
a	6.19	13
b	4.20	15
c	2.0	

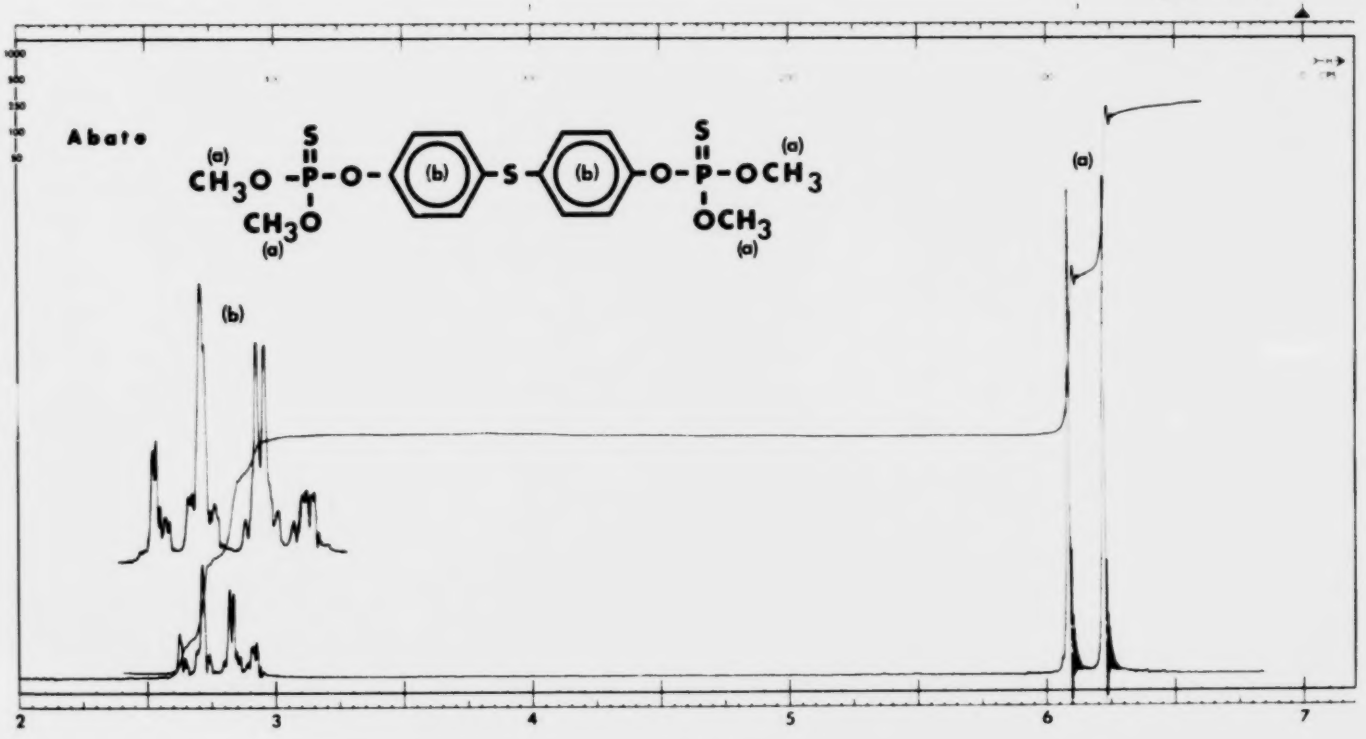
A-17

	T	J
a	6.23	15
b	4.98	15
c	2.18	



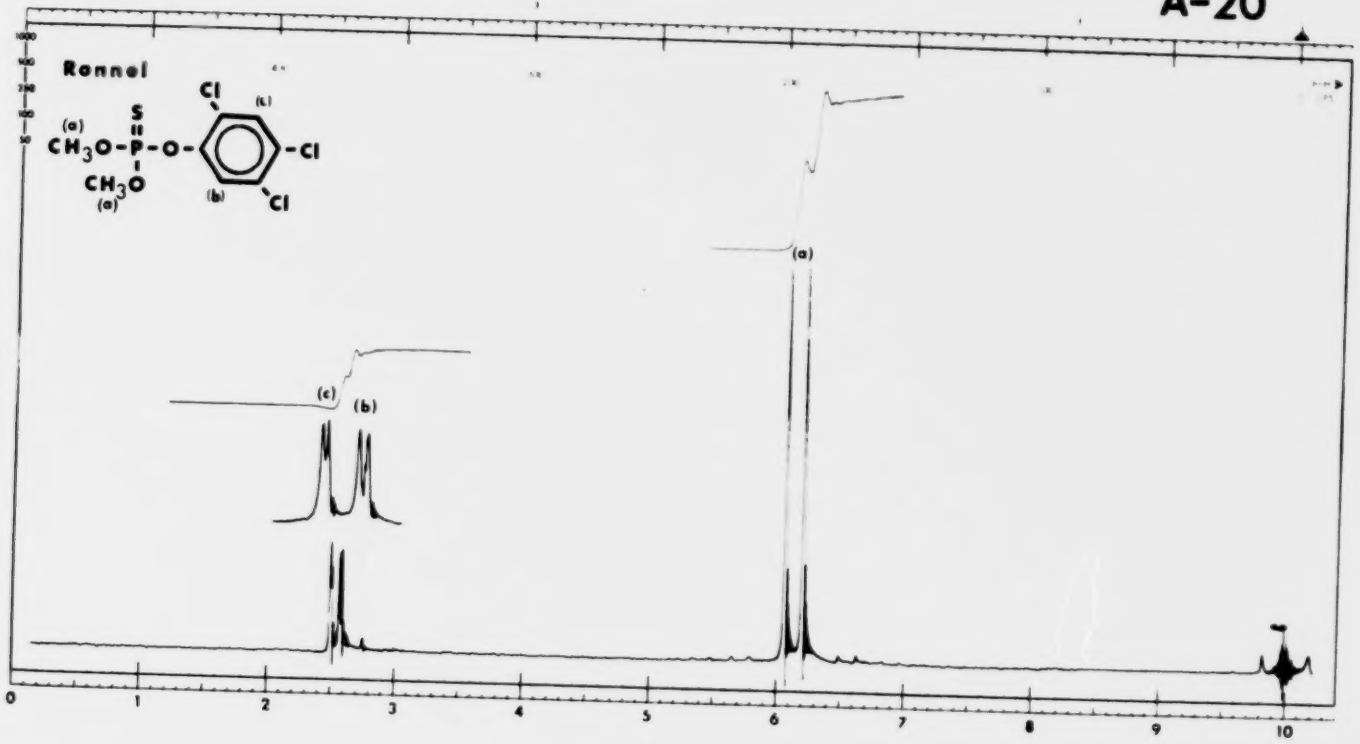
	T	J
a	7.68	
b	7.60	
c	6.19	14
d	3.0	

A-19

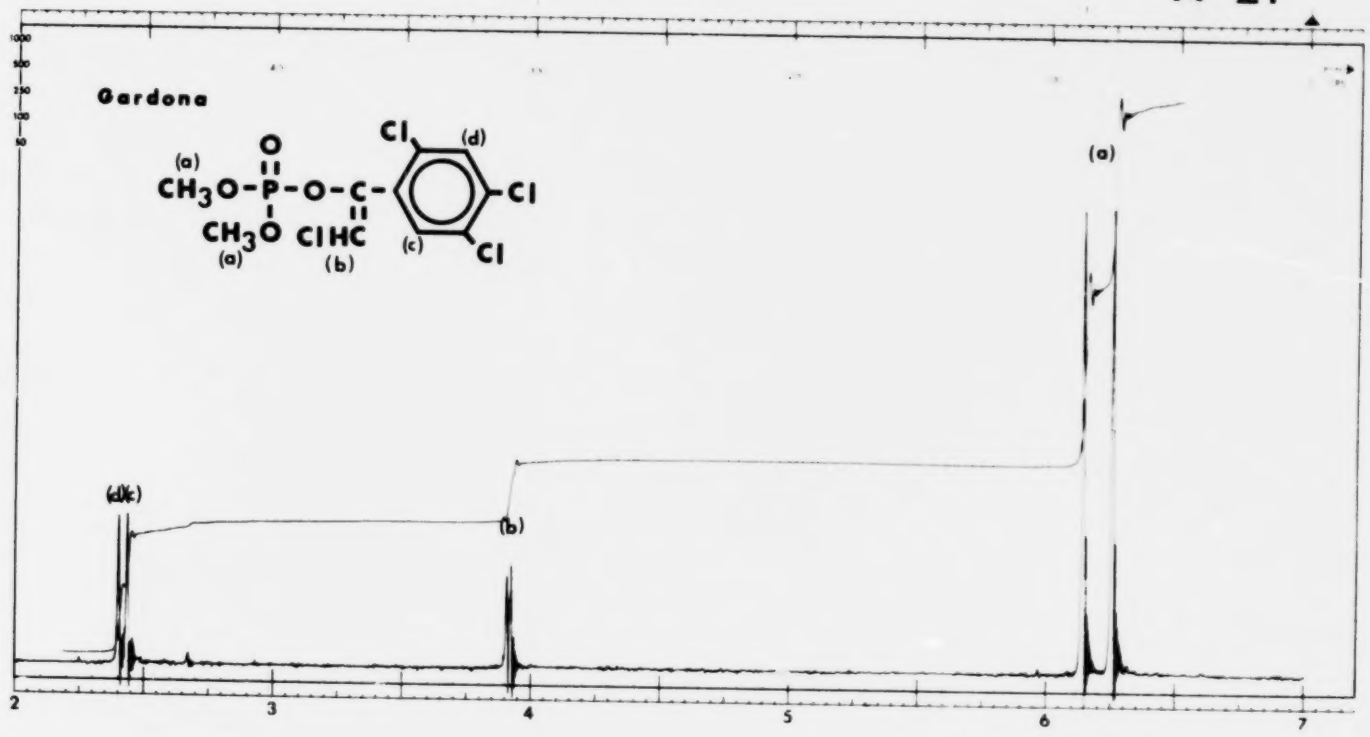


	T	J
a	6.17	14 (P-H)
b	2.5	

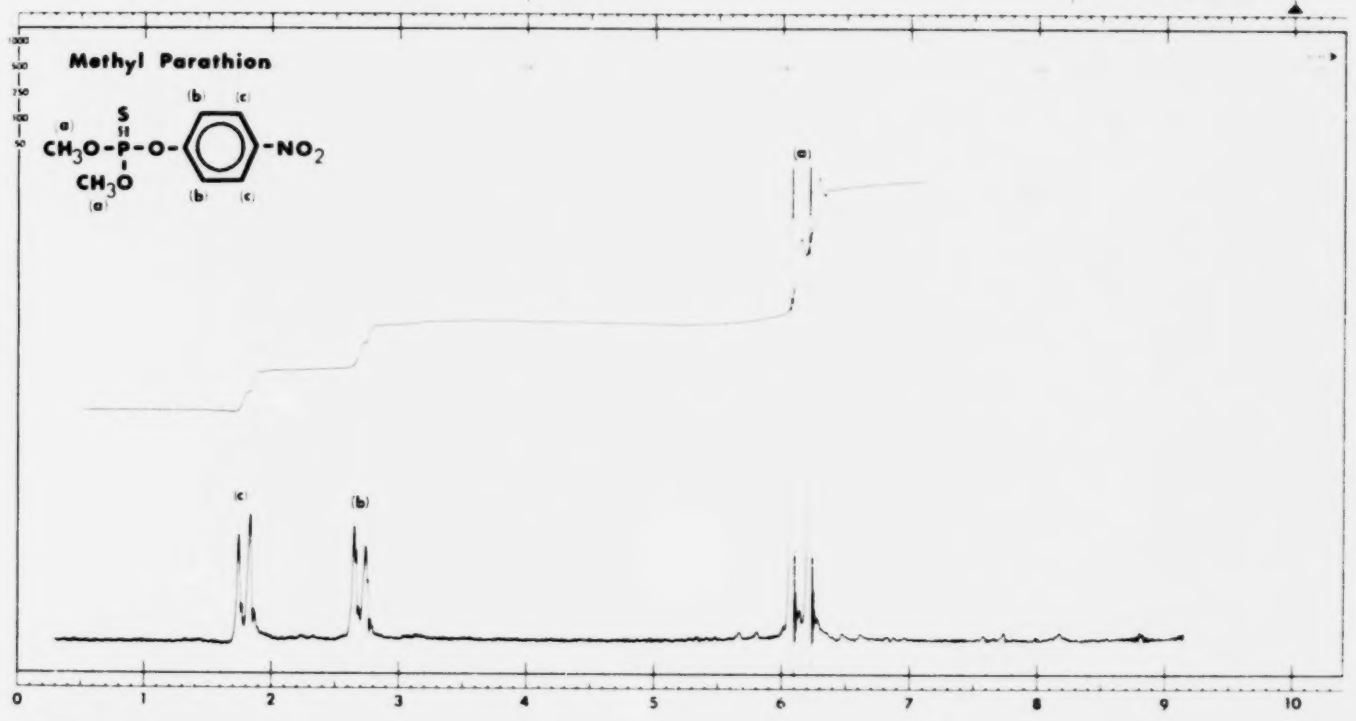
A-20



	T	J
a	6.10	14
b	2.55	1.8(P-H)
c	2.47	1.0(P-H)

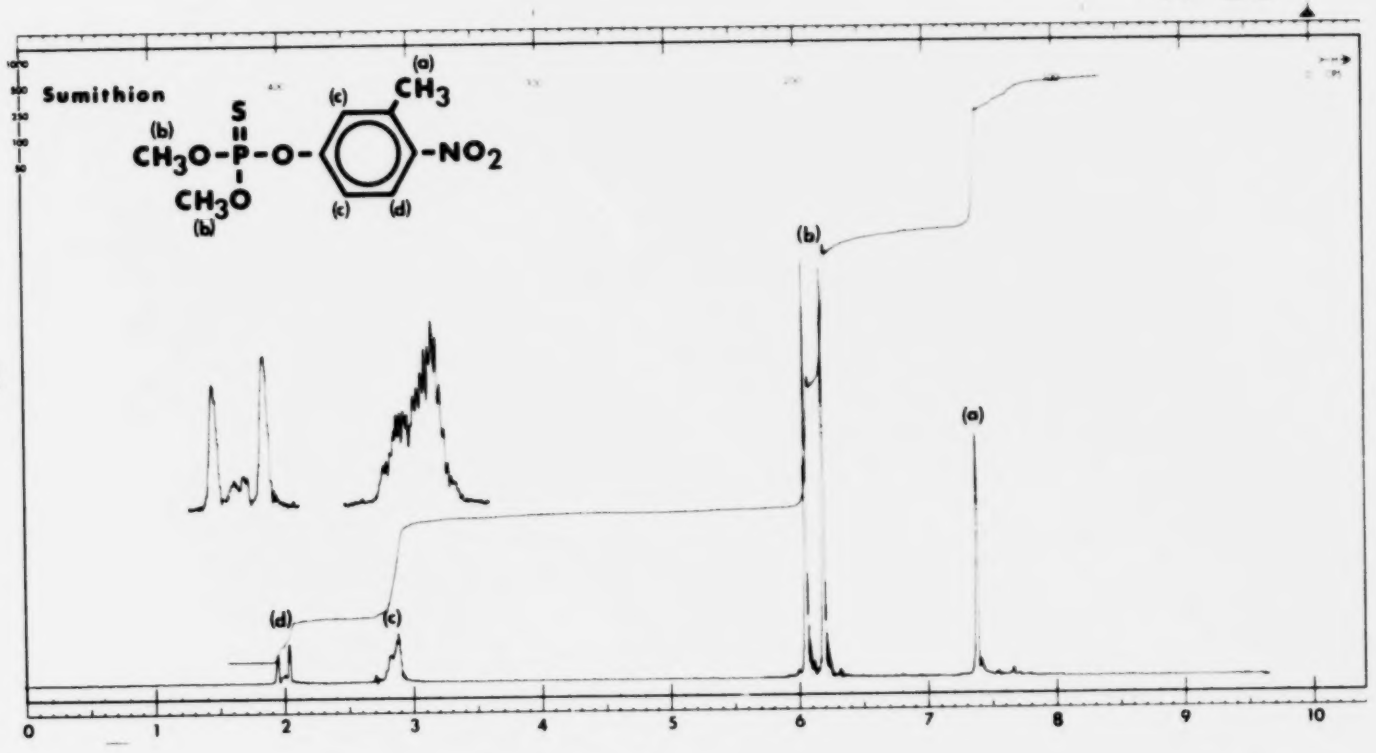


	T	J
a	6.21	11 (P-H)
b	3.92	1.5 (P-H)
c	2.46	
d	2.43	

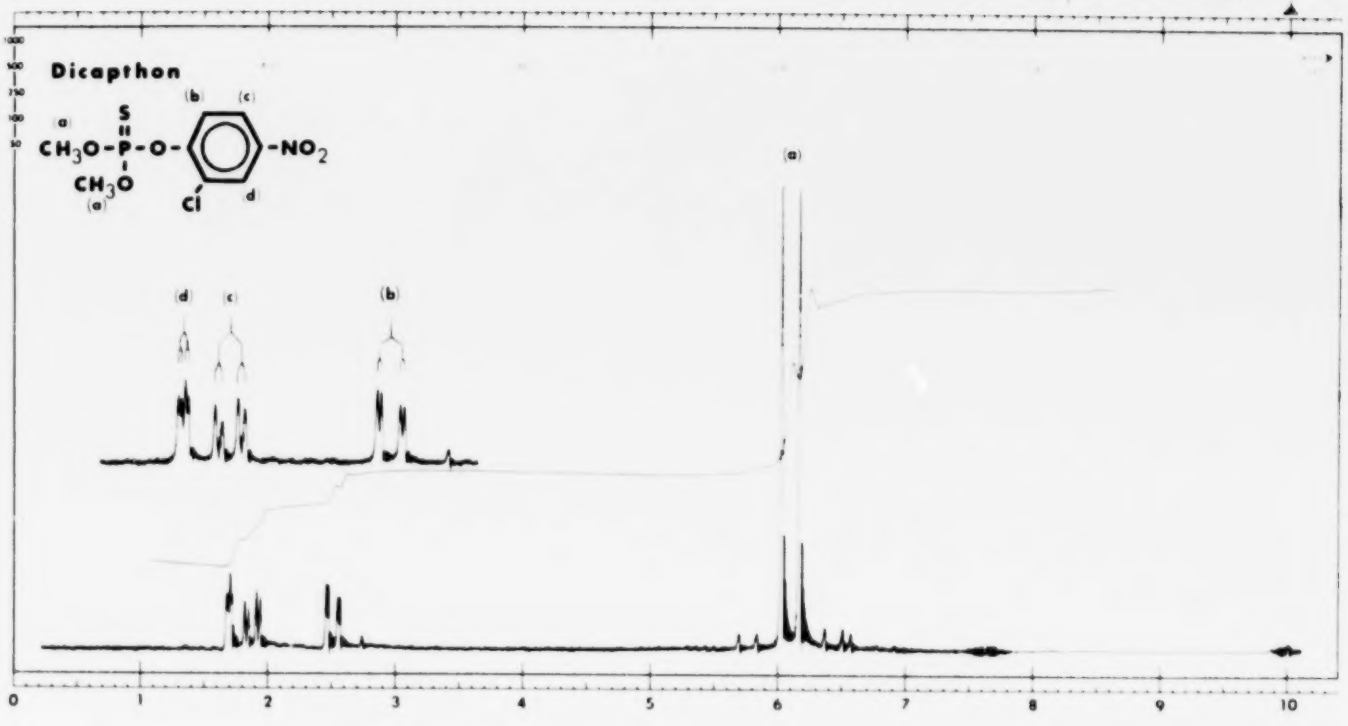


	T	J
a	6.13	14
b	2.70	9
c	1.78	9

A-23

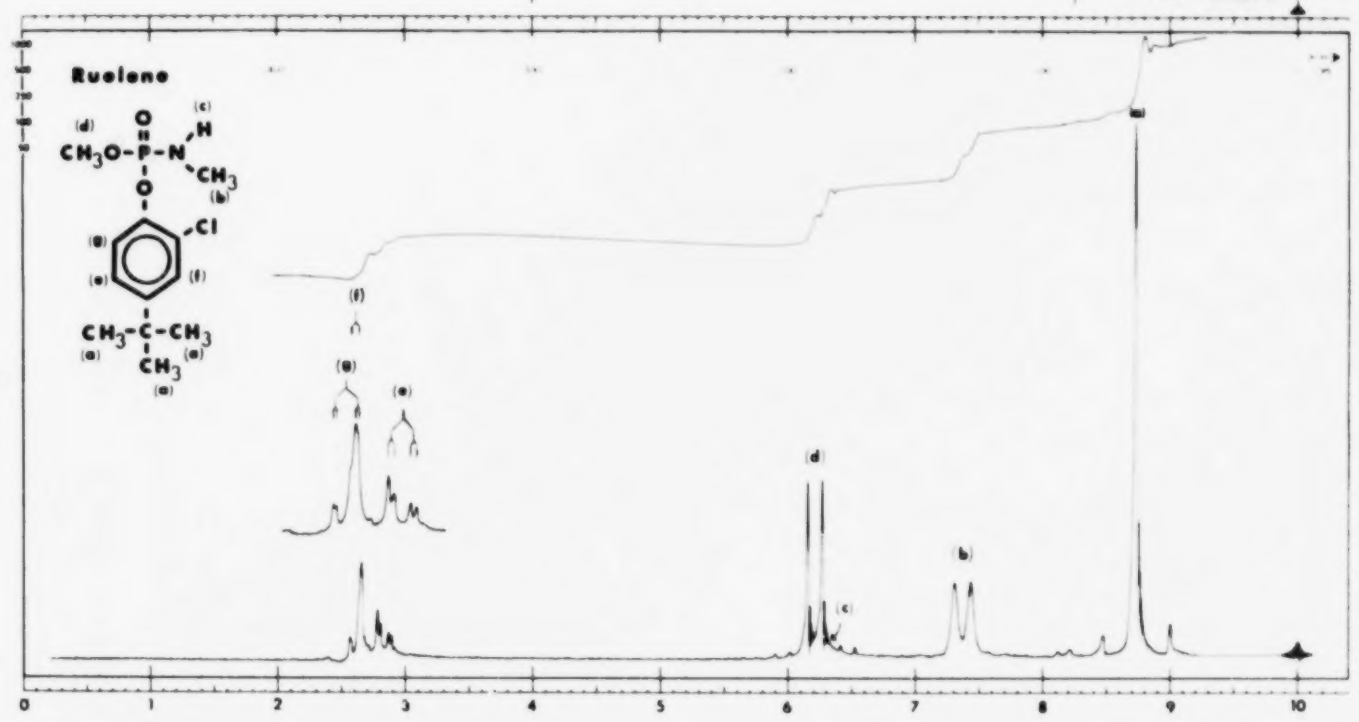


	T	J
a	7.38	
b	6.12	14 (P-H)
c	2.84	
d	1.98	

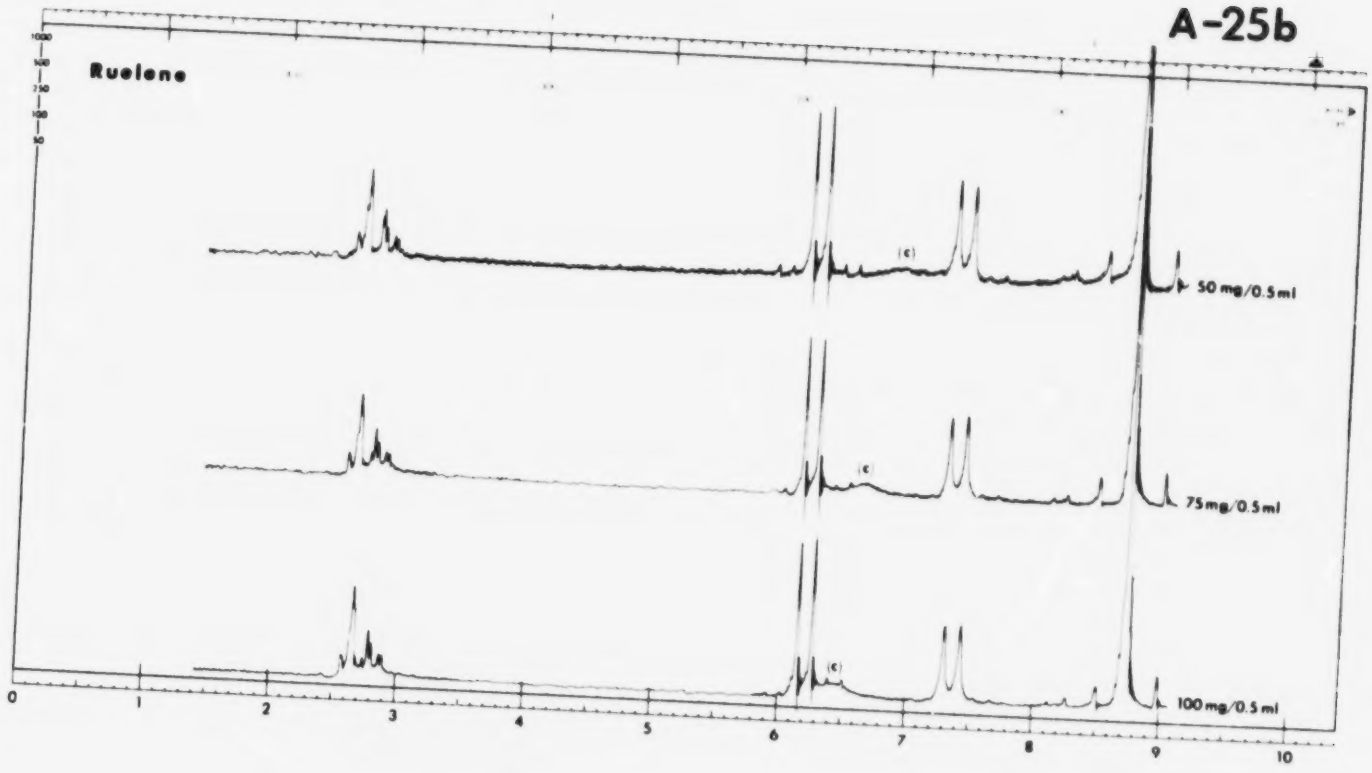


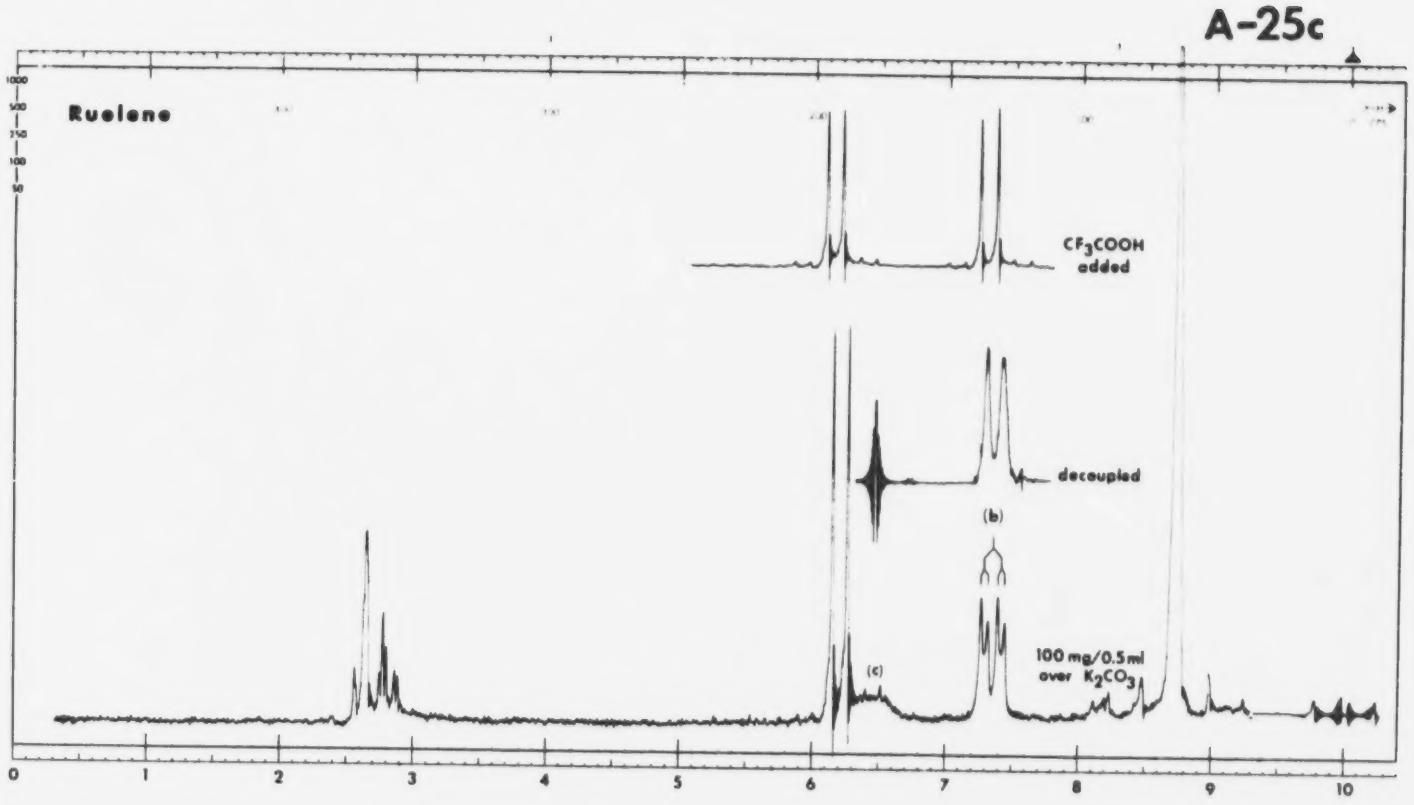
	T	J
a	6.08	14
b	2.49	9 H-Ho 1.5 P-H
c	1.87	9 H-Ho 2.8 H-Hm
d	1.68	2.8 H-Hm 12 P-H

A-25a

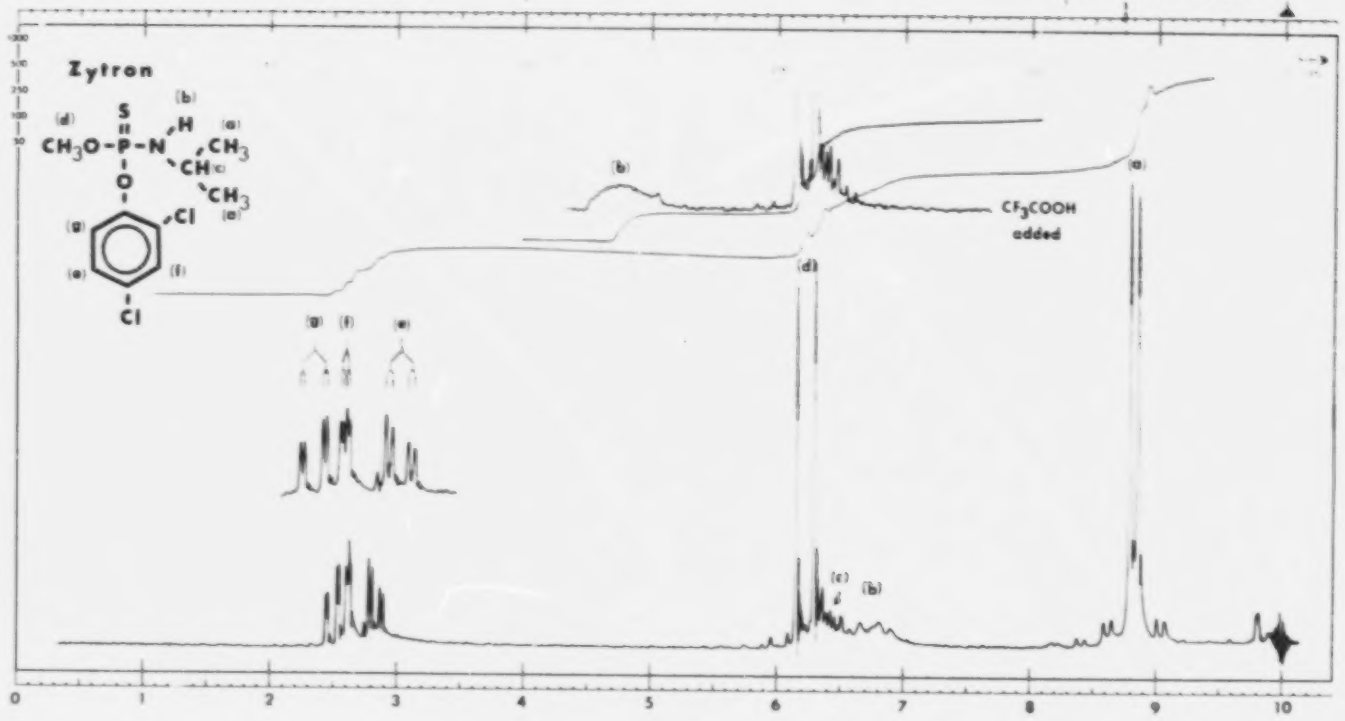


	T	J
a	8.72	
b	7.34	13 (P-H) 5 (H-H)
c	6.2-6.7	
d	6.19	11 (P-H)
e	2.80	9 ($H-H_o$) 2.5 ($H-H_m$)
f	2.62	2.5 ($H-H_m$)
g	2.57	9 ($H-H_o$) 1.0 ($P-H'$)

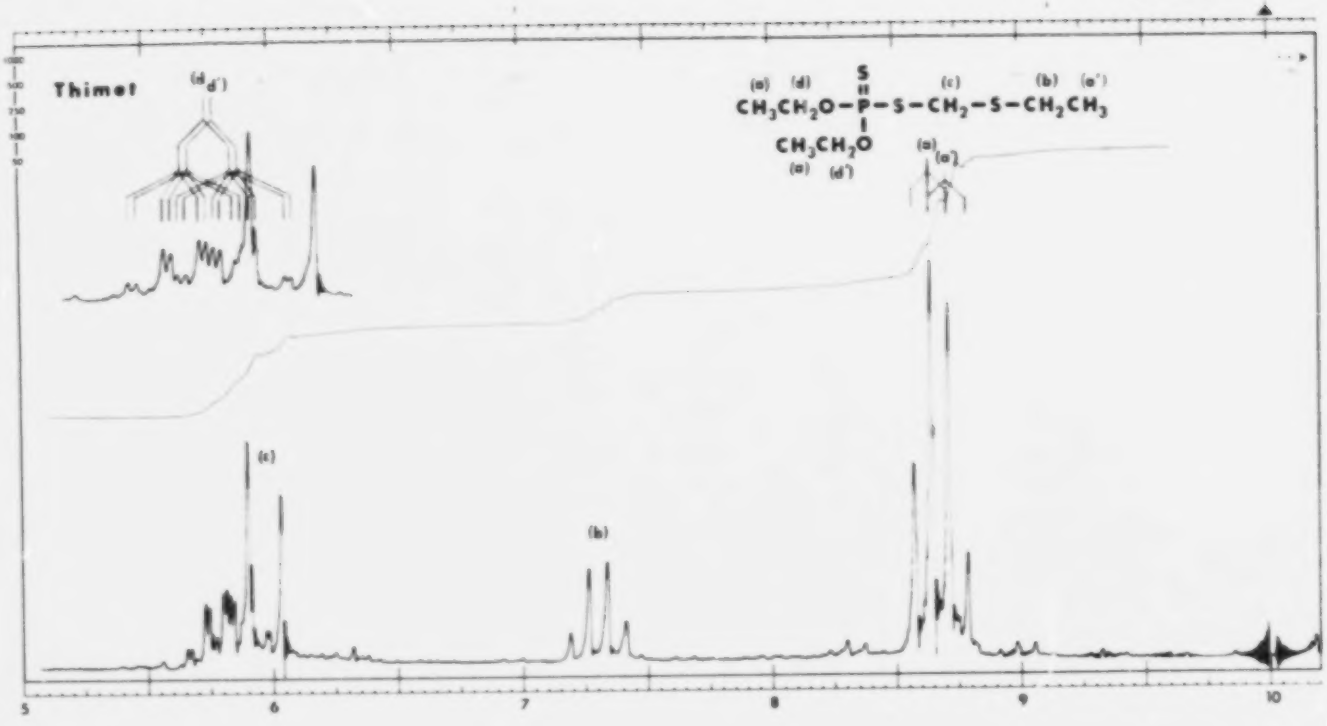

A-25b
Ruelene
50 mg/0.5 ml
75 mg/0.5 ml
100 mg/0.5 ml
0
1
2
3
4
5
6
7
8
9
10


A-25c
Ruelene
CF_3COOH added
decoupled
(b)
(c)
100 mg/0.5 ml over K_2CO_3
0
1
2
3
4
5
6
7
8
9
10

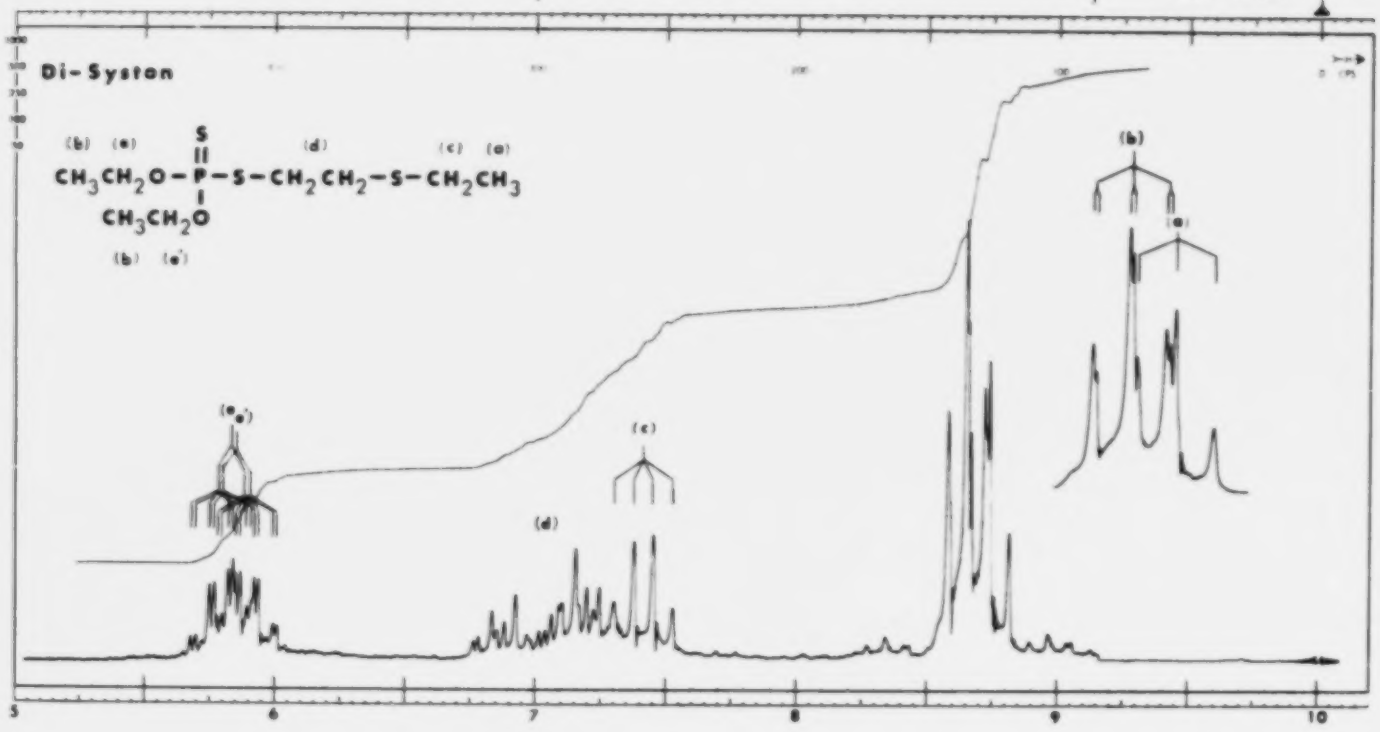
A-26



	T	J
a	8.81	6.5
b	6.8	
c	6.3	
d	6.20	14
e	2.81	9 (H-H_o) 2.5 (H-H_m)
f	2.59	2.5 (H-H_m) 1.0 (P-H)
g	2.46	9 (H-H_o) 1.3 (P-H)

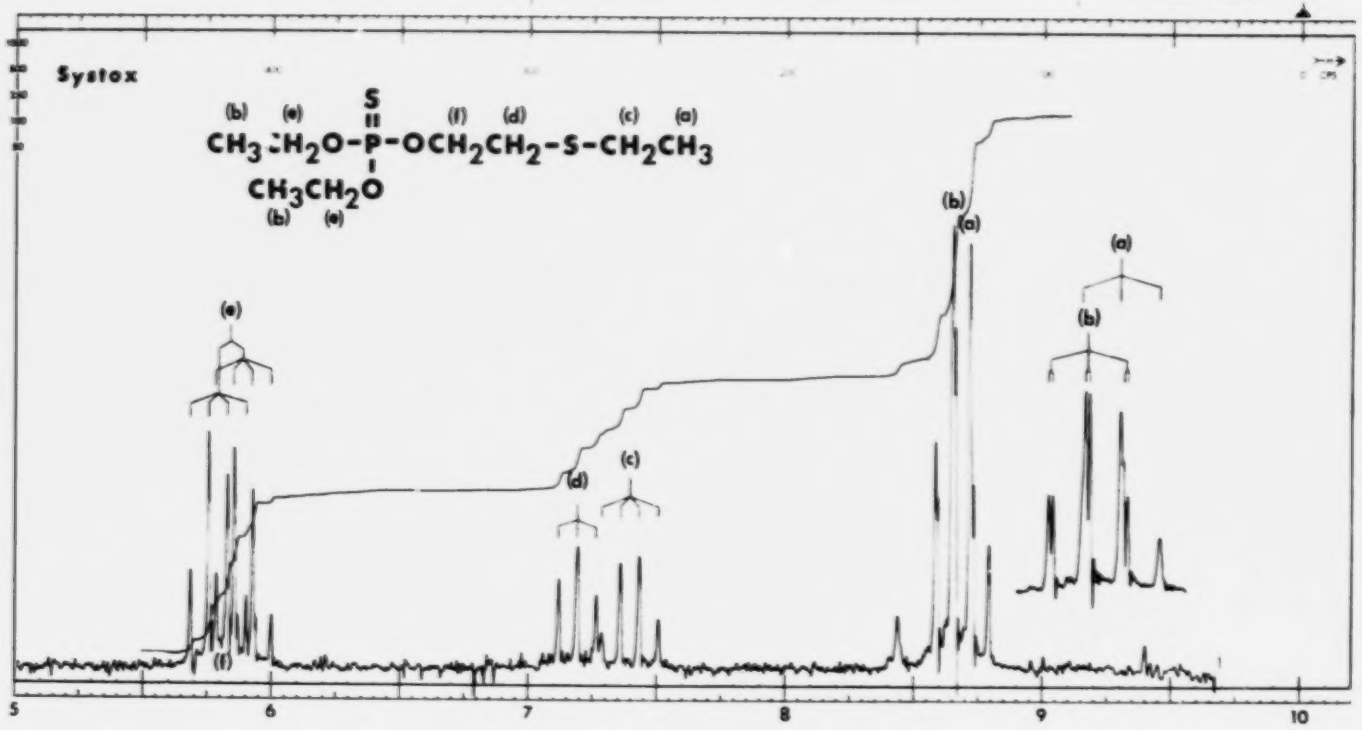


	T	J
a	8.64	7 (H-H) 0.8 (P-H)
a'	8.71	7
b	7.30	7
c	5.97	13 (P-H)
d	5.815	10 (P-H)
d'	5.83	7 (H-H)



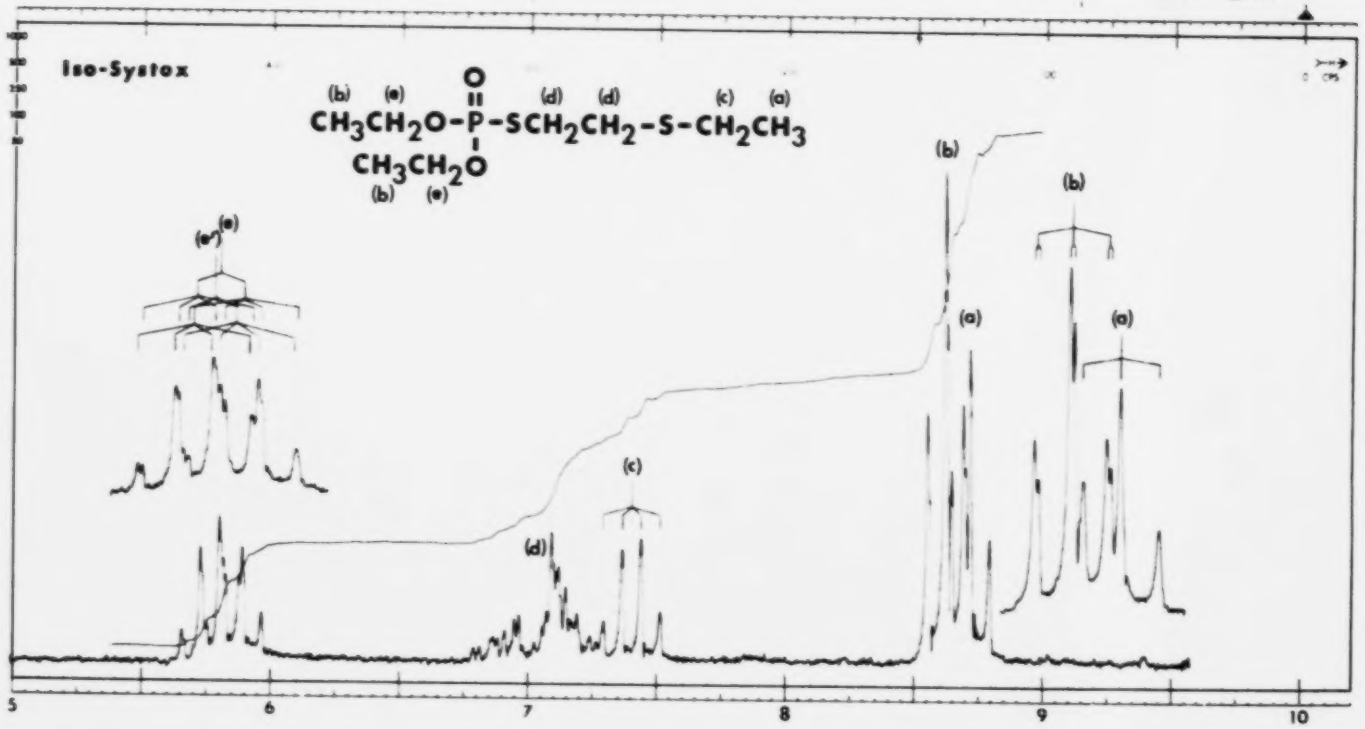
	T	J
a	8.73	7.5
b	8.65	7 (H-H) 0.7 (P-H)
c	7.40	7.5
d	6.5-7.5	
a	5.83	10 (P-H)
a'	5.85	7 (H-H)

A-29



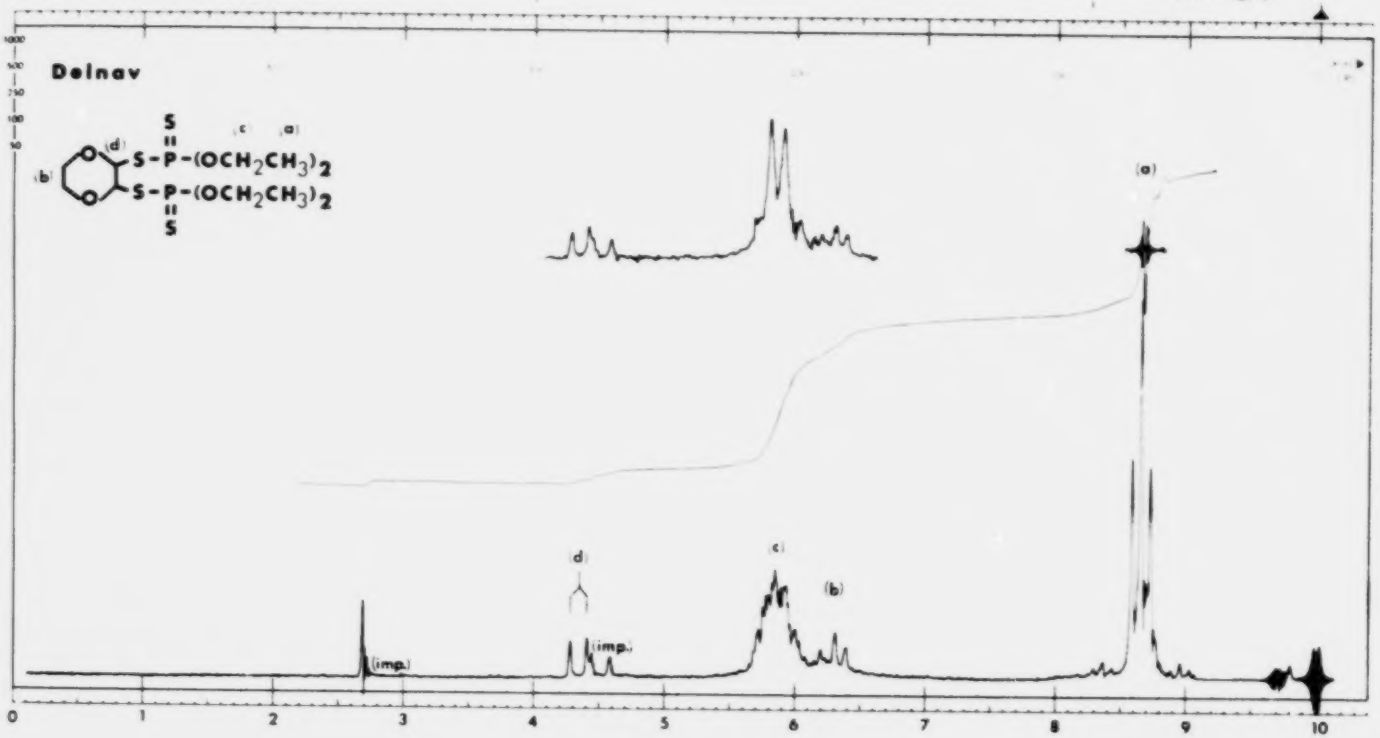
	T	J
a	8.73	7.5
b	8.67	7 (H-H), 0.9 (P-H)
c	7.41	7.5
d	7.20	7
e	5.86	7 (H-H), 10 (P-H)
f	5.8	

A-30

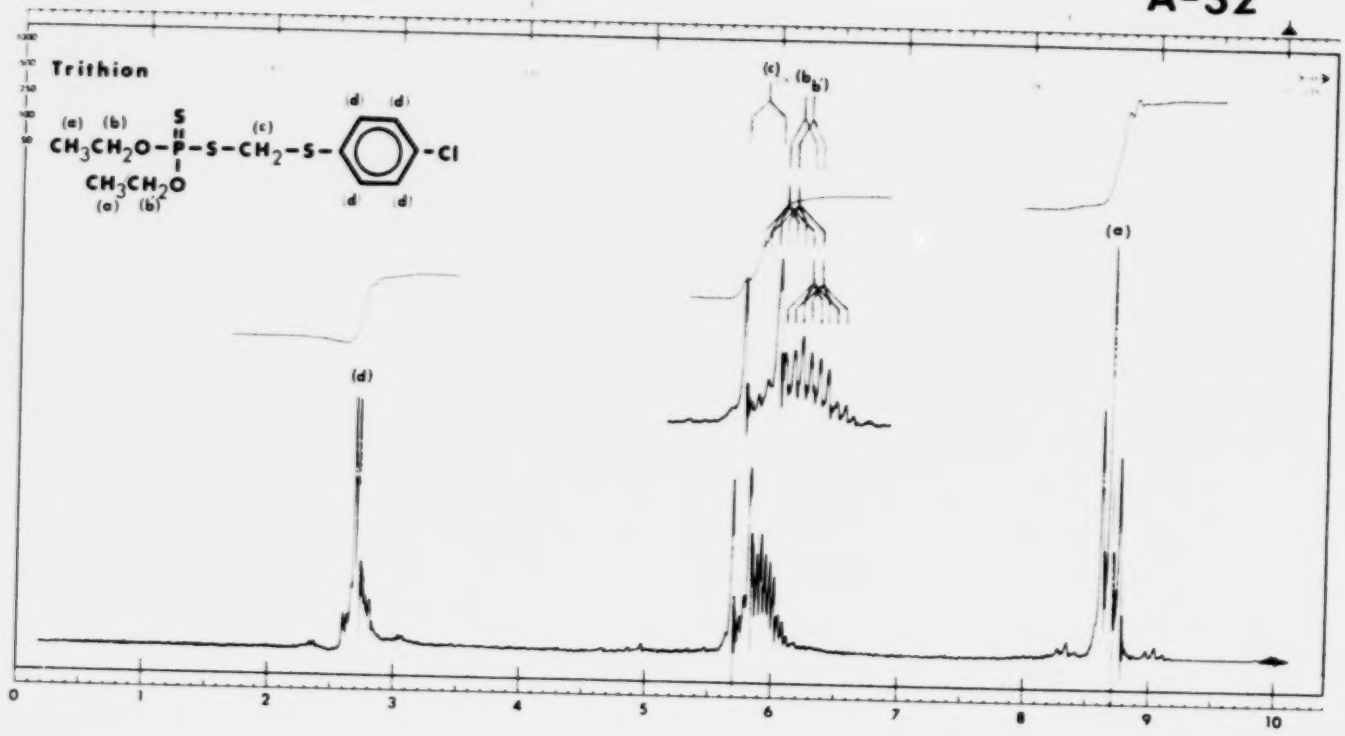


	T	J
a	8.73	7.5
b	8.62	7 (H-H), 0.9 (P-H)
c	7.40	7.5
d	7.0	
e	5.82	7 (H-H)
e	5.81	9 (P-H)

A-31

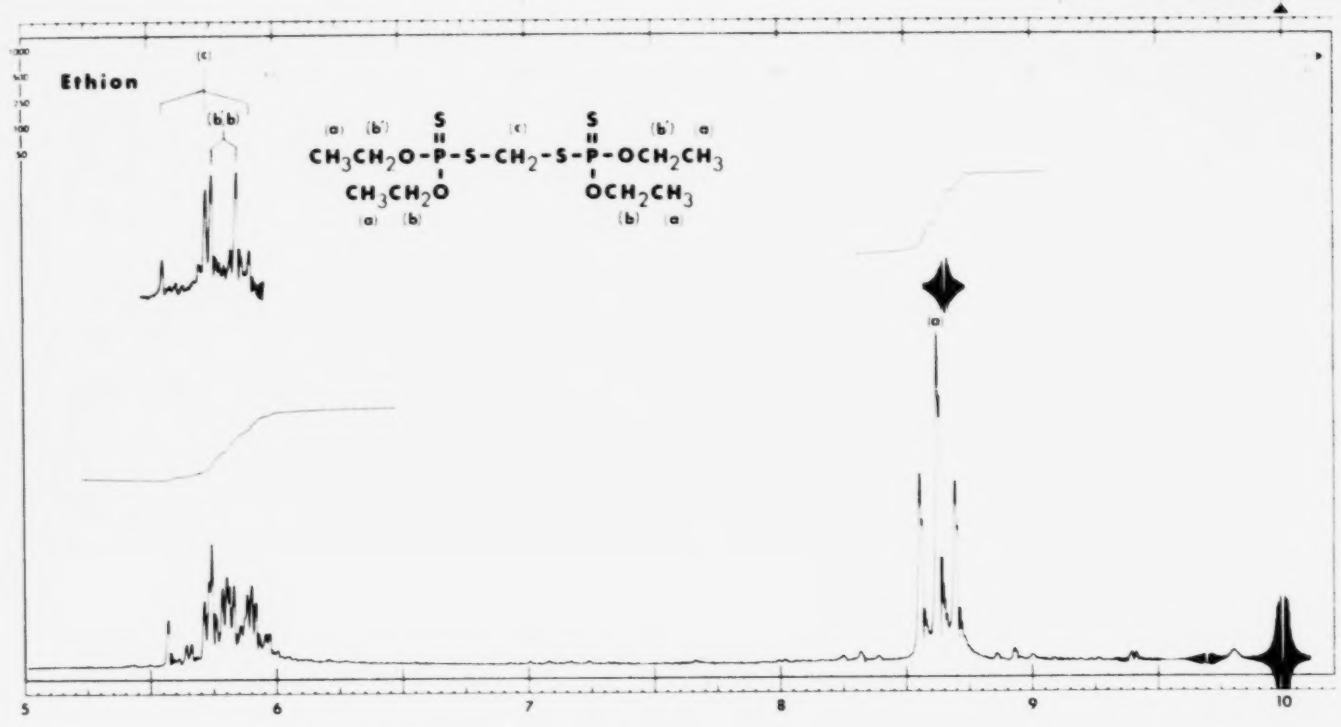


	T	J
a	8.64	7
b	6.3	
c	5.83	10 (P-H)
d	4.32	13



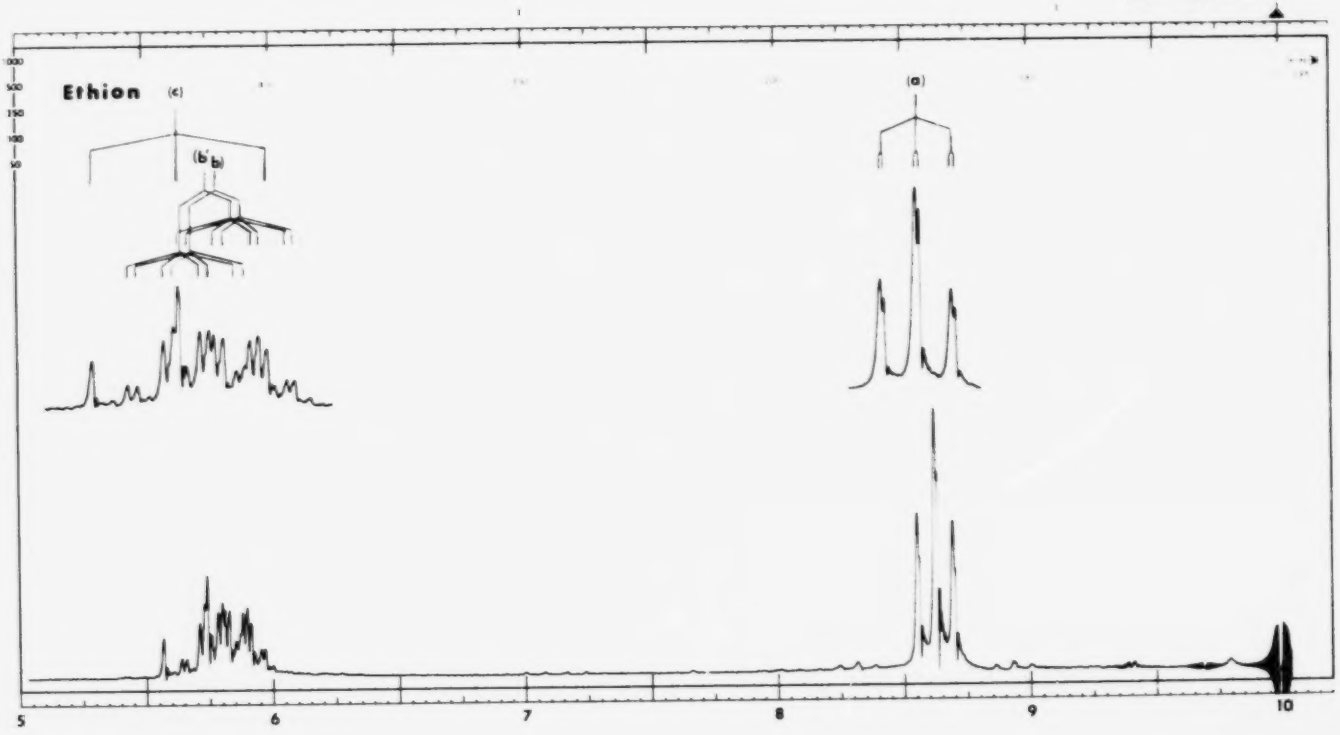
	T	J
a	8.67	7
b	5.88	10(P-H)
b	5.91	7 (H-H)
c	5.72	13.5(P-H)
d	2.68	

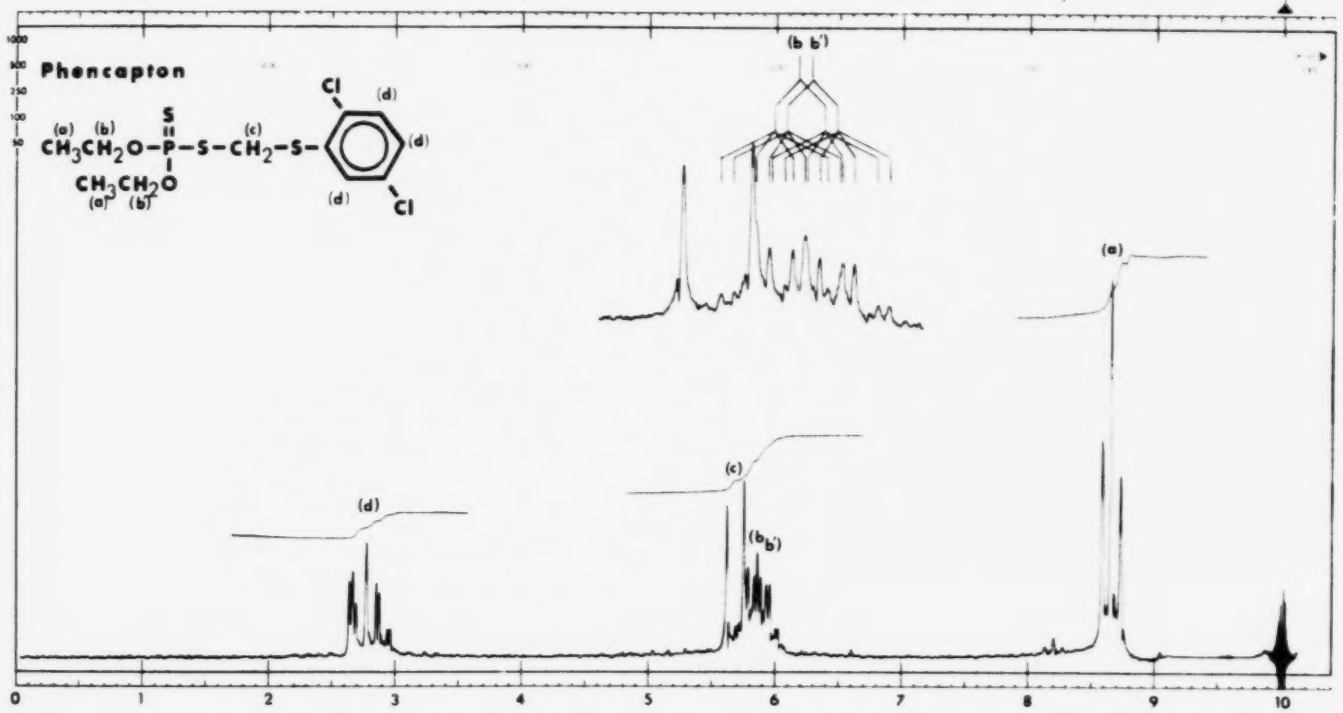
A-33a



	T	J
a	8.62	7 H-H 0.8 P-H
b	5.82	7 H-H 10 P-H
b'	5.80	7 H-H 10 P-H
c	5.74	17 P-H

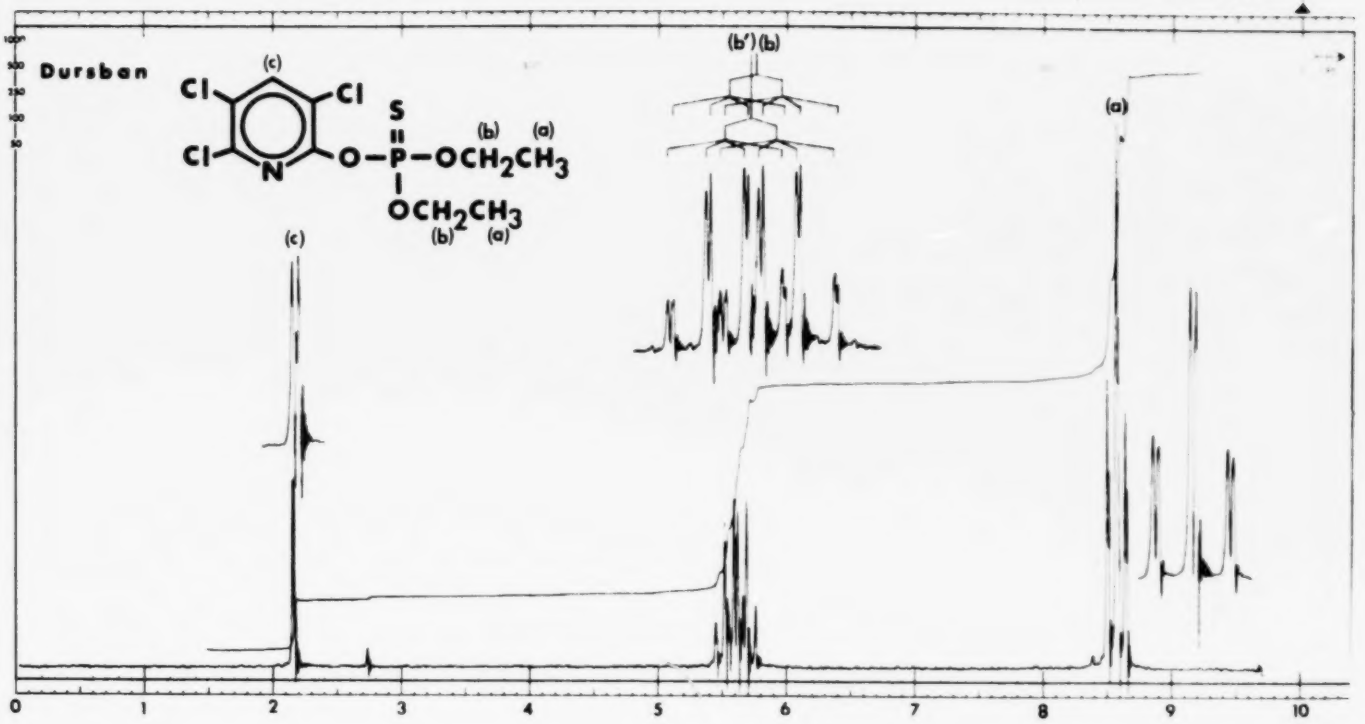
A-33b



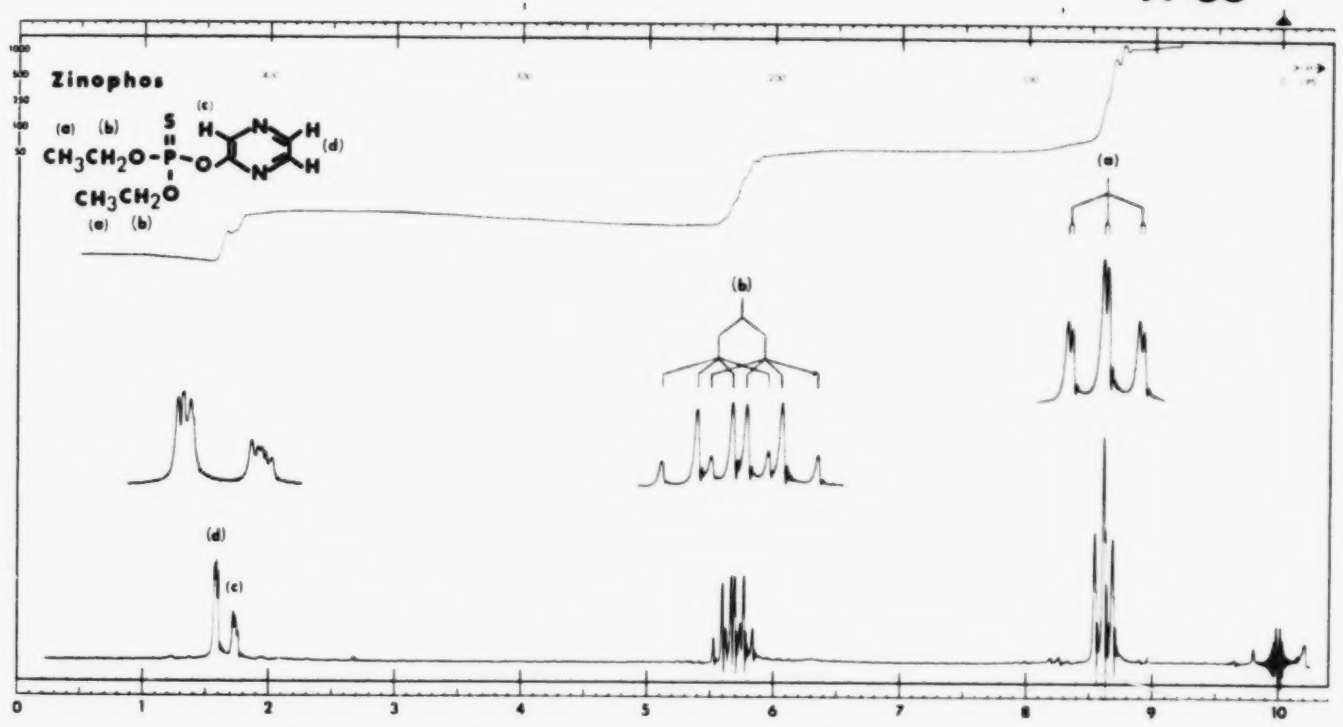


	T	J
a	8.64	7
b	5.82	10 (P-H)
b'	5.84	7 (H-H)
c	5.66	14
d	2.8	

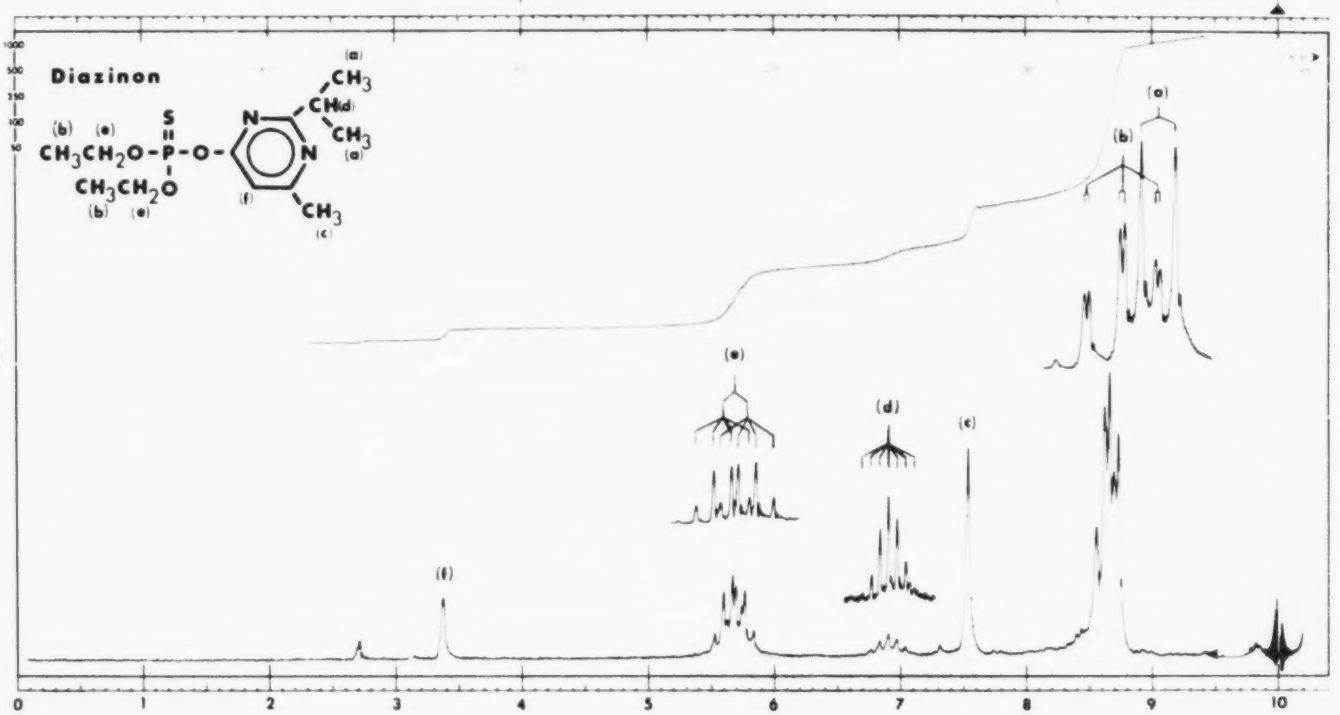
A-35



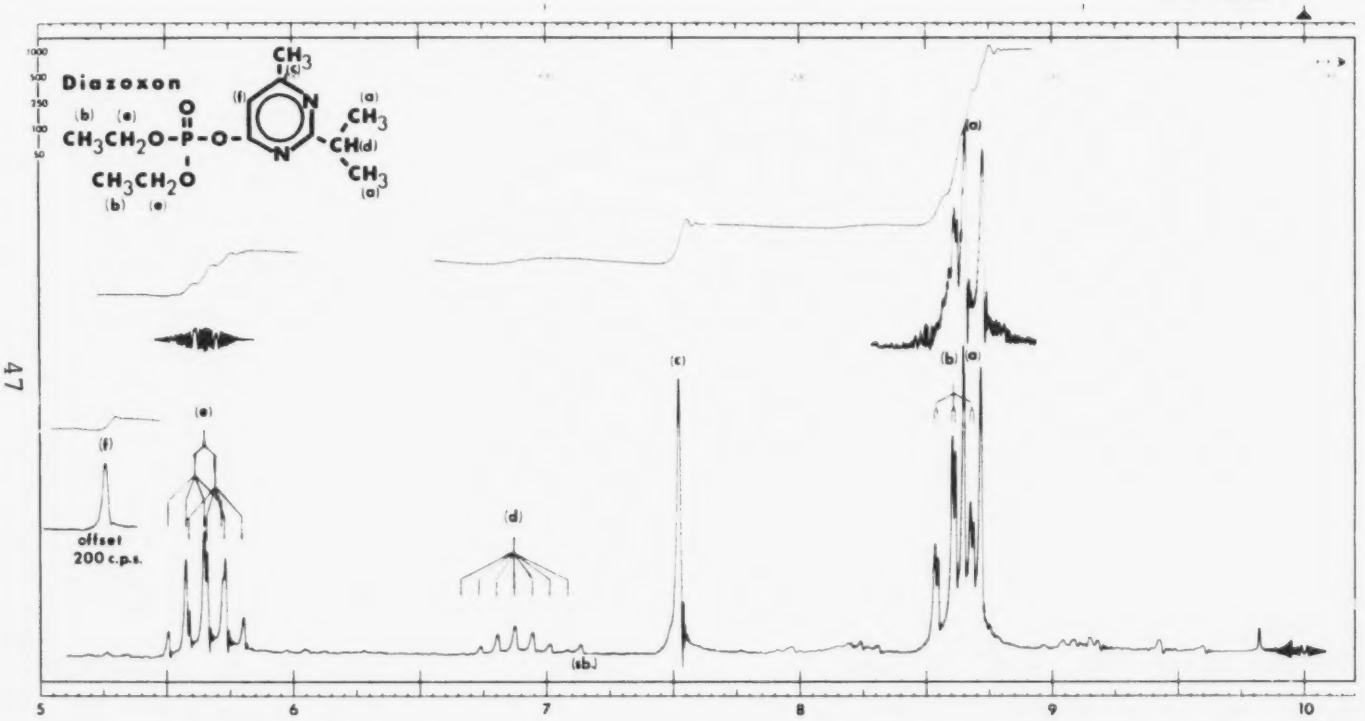
	T	J
a	8.59	7 (H-H), 1 (P-H)
b	5.61	7 (H-H), 10 (P-H)
b'	5.60	
c	2.16	1.2 (P-H)



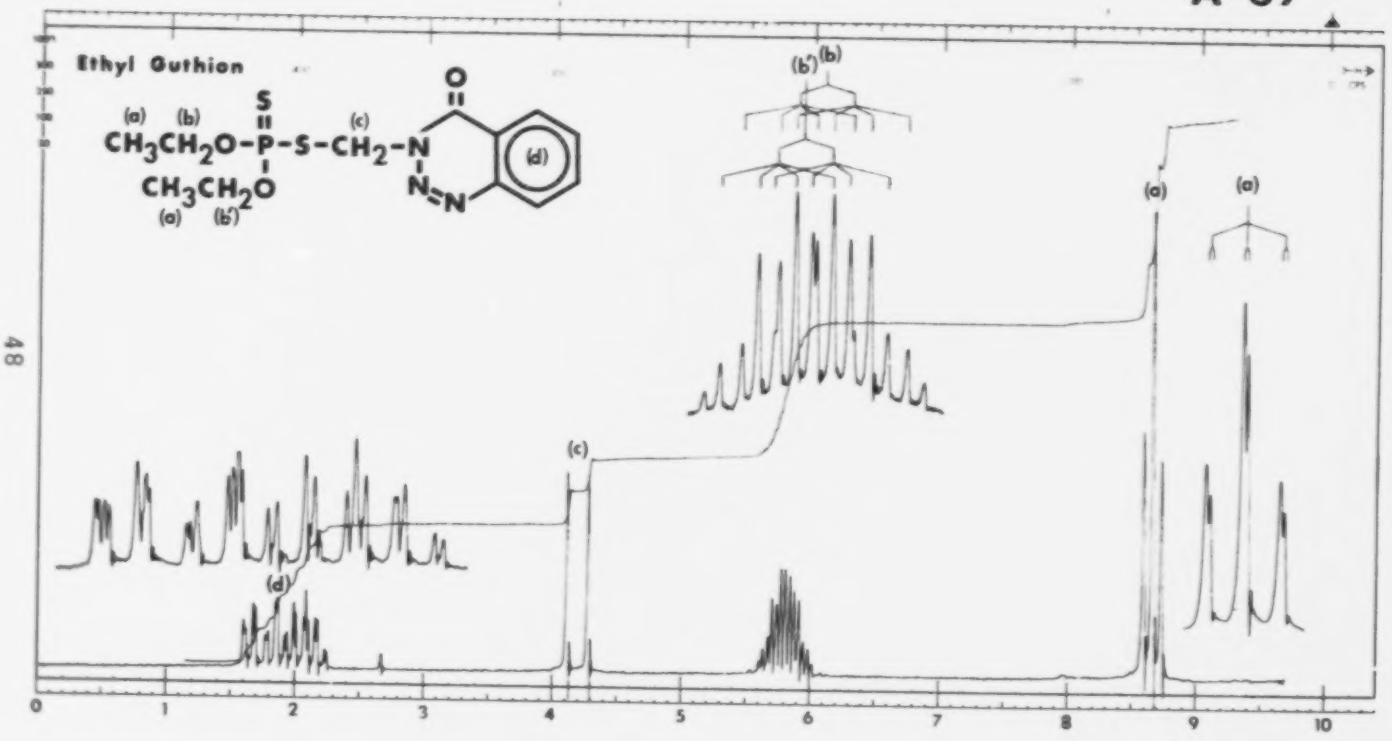
	T	J
a	8.59	7 (H-H) 0.8 (P-H)
b	5.65	9 (P-H) 7 (H-H)
c	1.72	
d	1.67	



	T	J
a	8.68	7
b	8.62	≤ 7 (H-H), ≤ 0.8 (P-H)
c	7.51	
d	6.88	7
e	5.66	≤ 9.5 (P-H), ≤ 7 (H-H)
f	3.34	

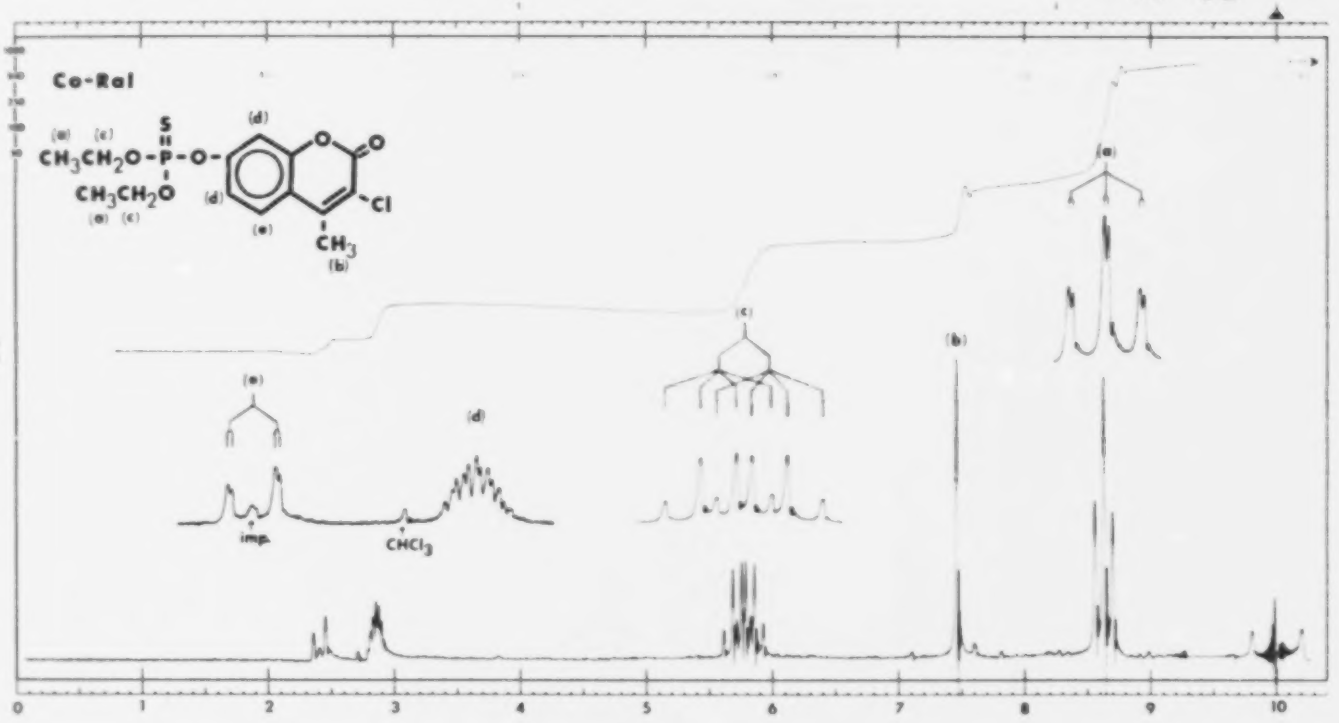


	T	J
a	8.68	7
b	8.61	7 (H-H) 1.2 (P-H)
c	7.51	
d	6.87	7
e	5.65	7 (H-H) 8 (P-H)
f	3.26	

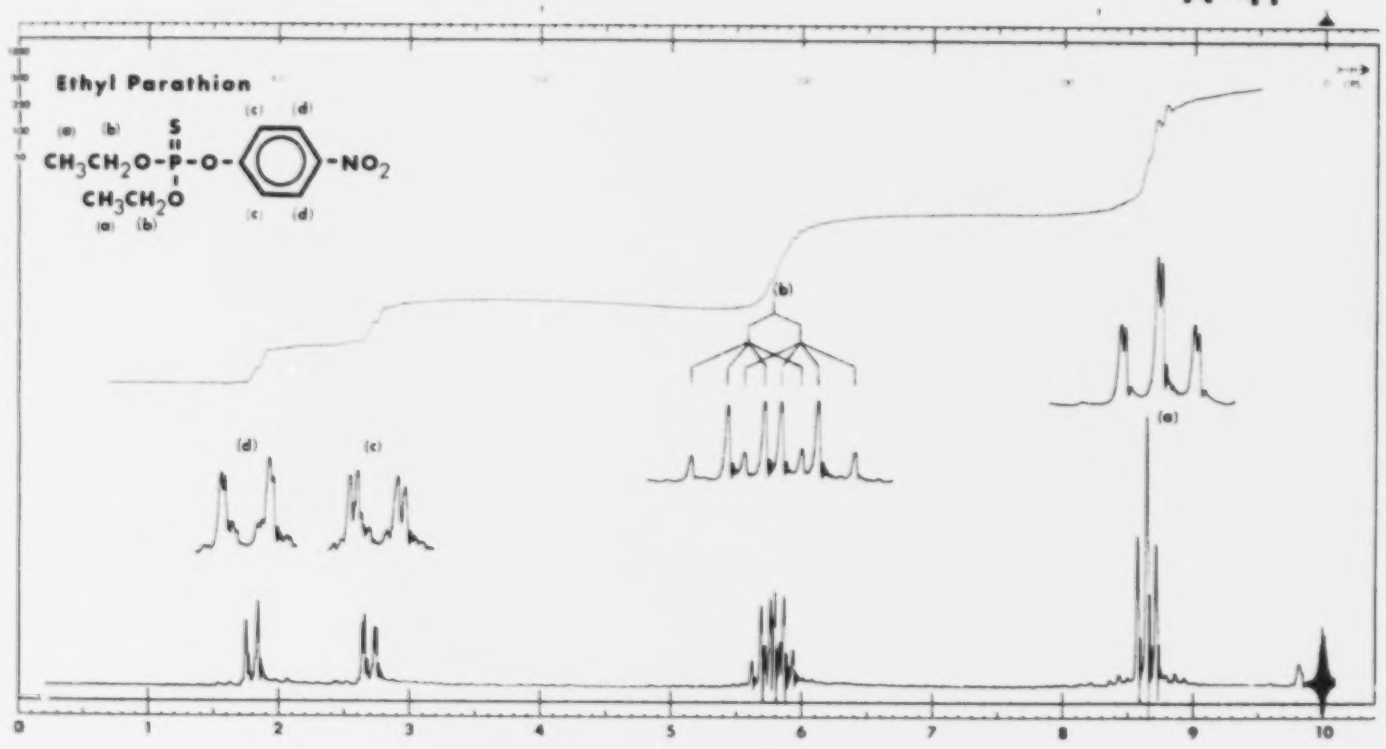


	T	J
a	8.66	0.8 (P-H), 7 (H-H)
b	5.84	10.5 (P-H), 7 (H-H)
b'	5.80	
c	4.19	16 (P-H)
d	1.9	

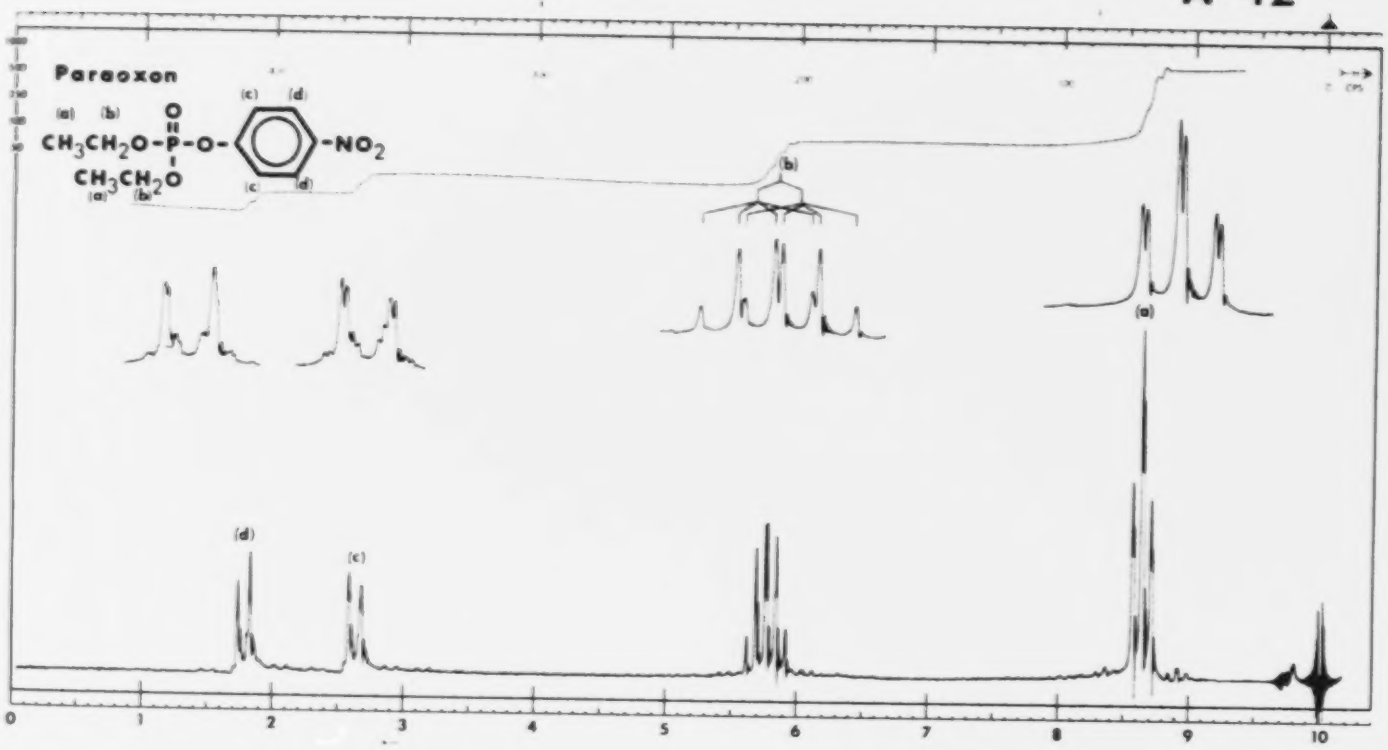
A-40



	T	J
a	8.60	7.0 (H-H) 0.8 (P-H)
b	7.43	
c	5.75	7.0 (H-H) 10.0 (P-H)
d	2.83	
e	2.37	9.5 (H-H_o) 0.8

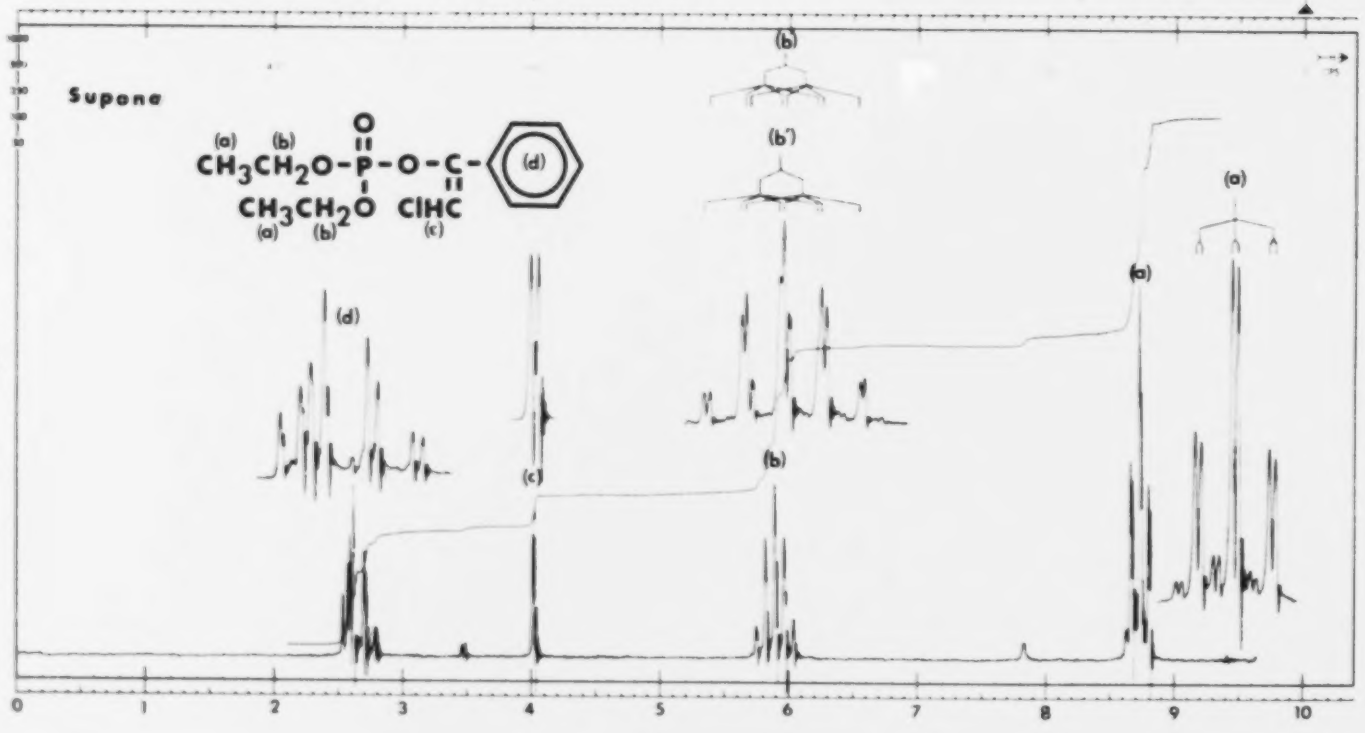


	T	J
a	8.63 <	0.8 (P-H) 7 (H-H)
b	5.75 <	10 (P-H) 7 (H-H)
c	2.67 <	9 (H-H) 1.3 (P-H)
d	1.77 <	9 (H-H) 0.7 (P-H)

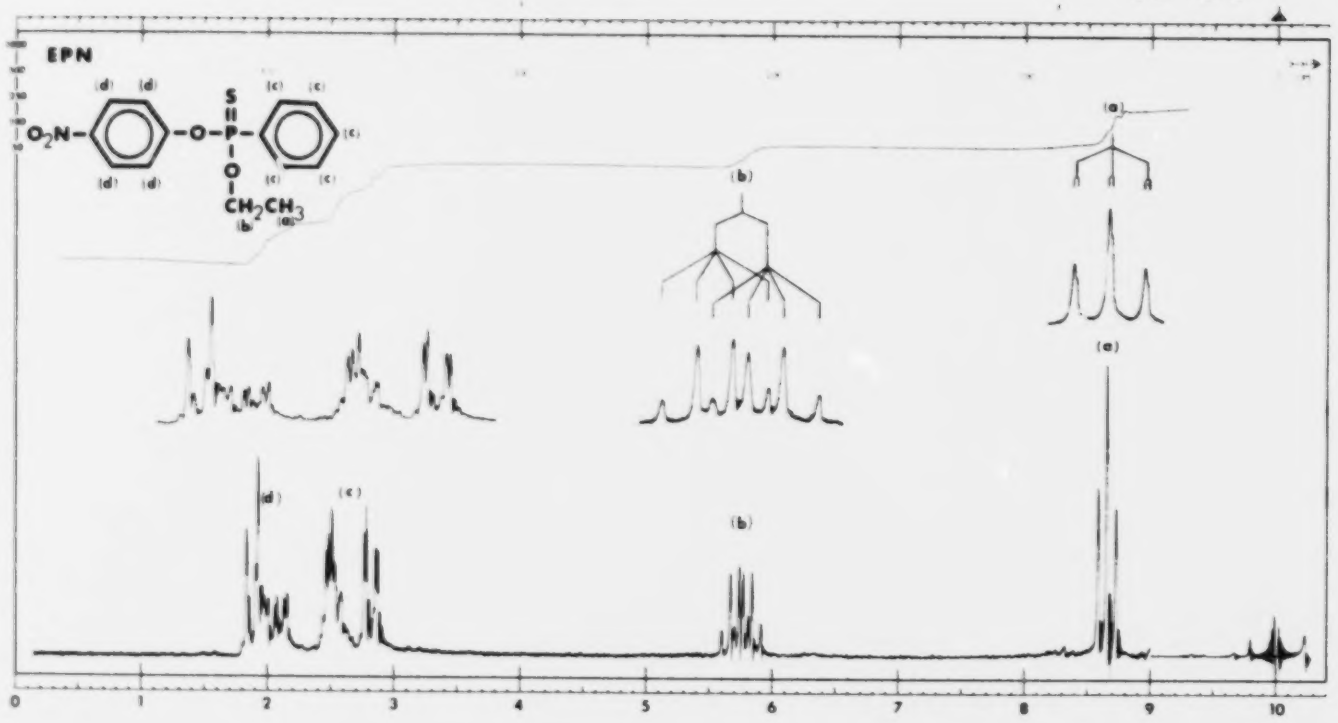


	T		J
a	8.61	<	7 (H-H) 0.9 (P-H)
b	5.74	<	8.5 (P-H) 7 (H-H)
c	2.60	<	9 (H-H) 1.0 (P-H)
d	1.78	<	9 (H-H) 0.7 (P-H)

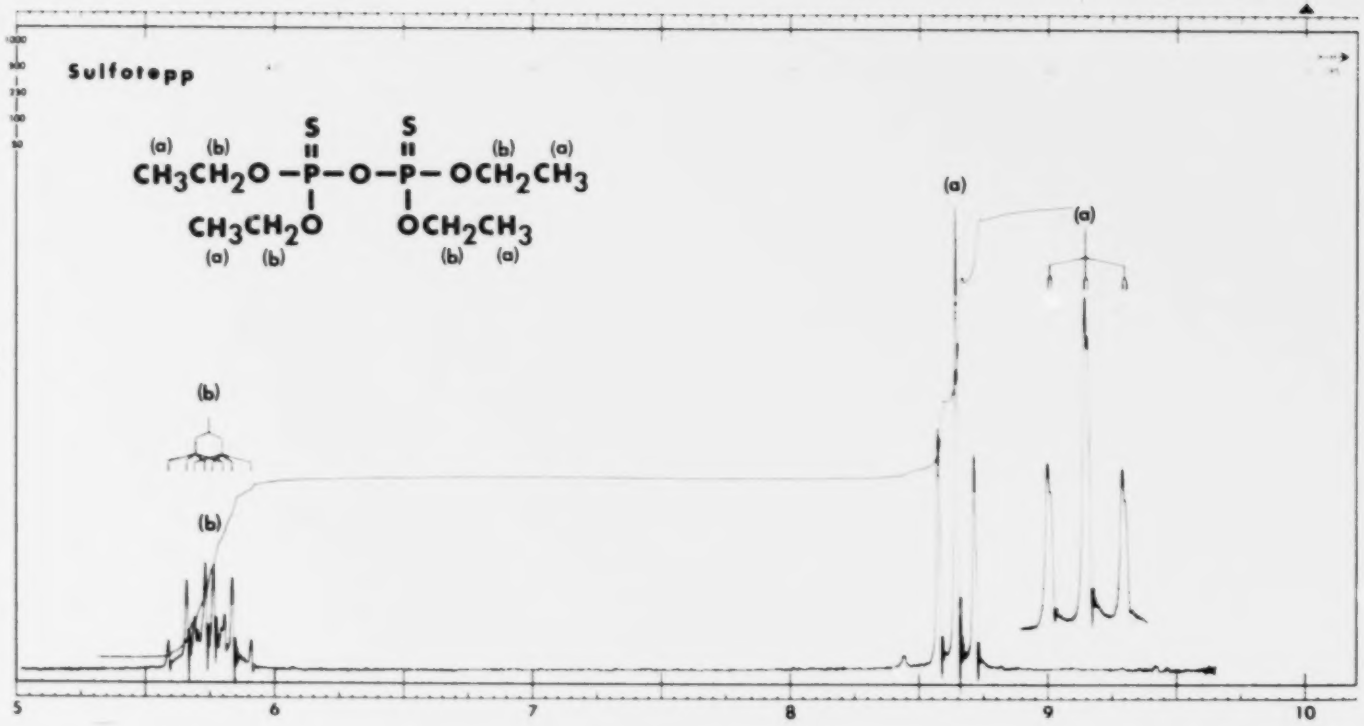
A-43



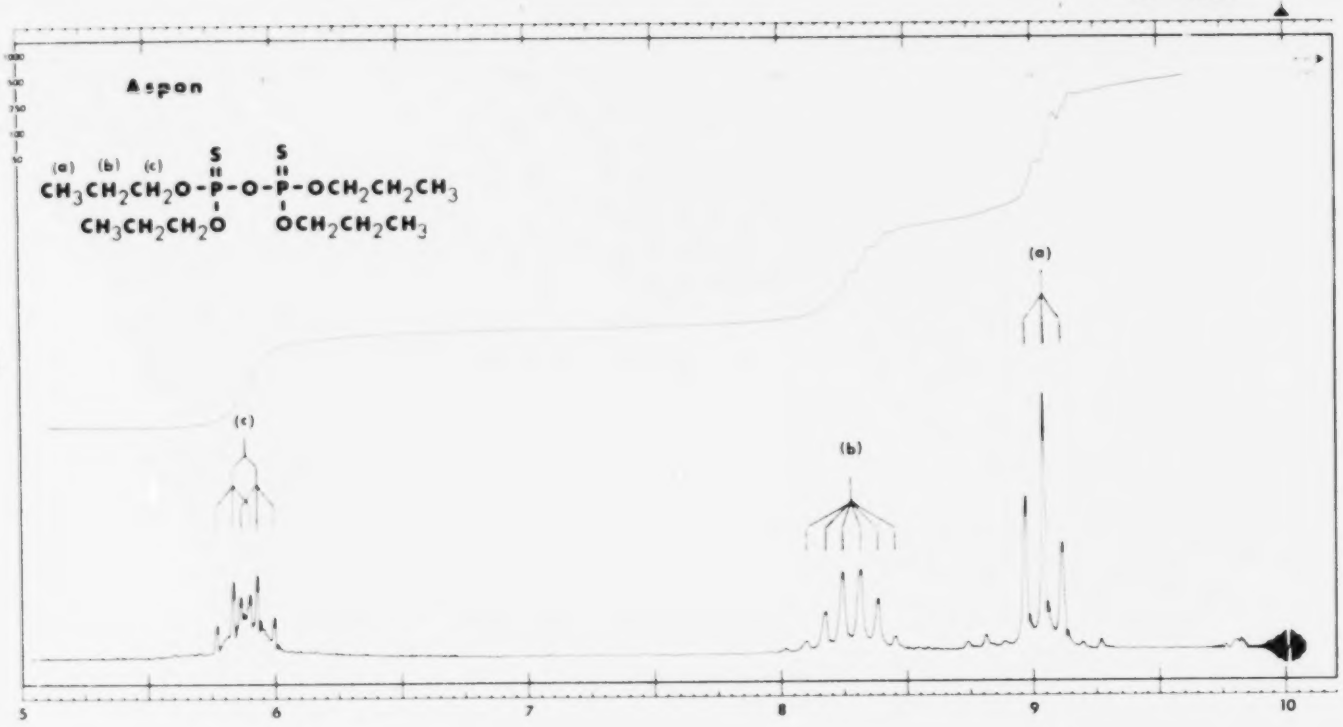
	T	J
a	8.74	7 / 1.2 (P-H)
b	5.89	7
b'	5.88	7
c	4.00	1.5 (P-H)
d	2.65	



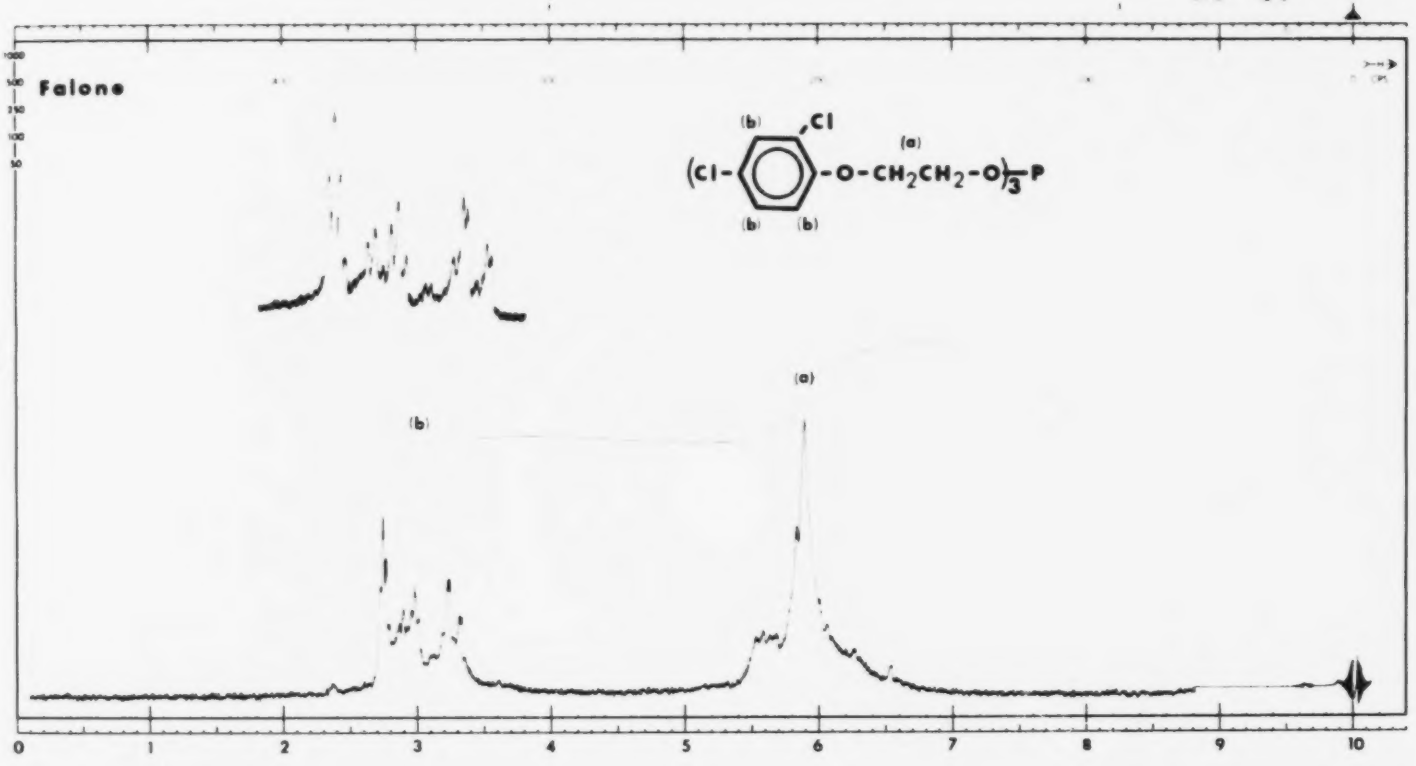
	T	J
a	8.64	< 7 (H-H) < 0.5 (P-H)
b	5.73	< 7 (H-H) < 10 (P-H)
c	2.64	
d	1.96	



	T	J
a	8.65	7 (H-H), 0.5 (P-H)
b	5.76	7 (H-H), 10 (P-H)

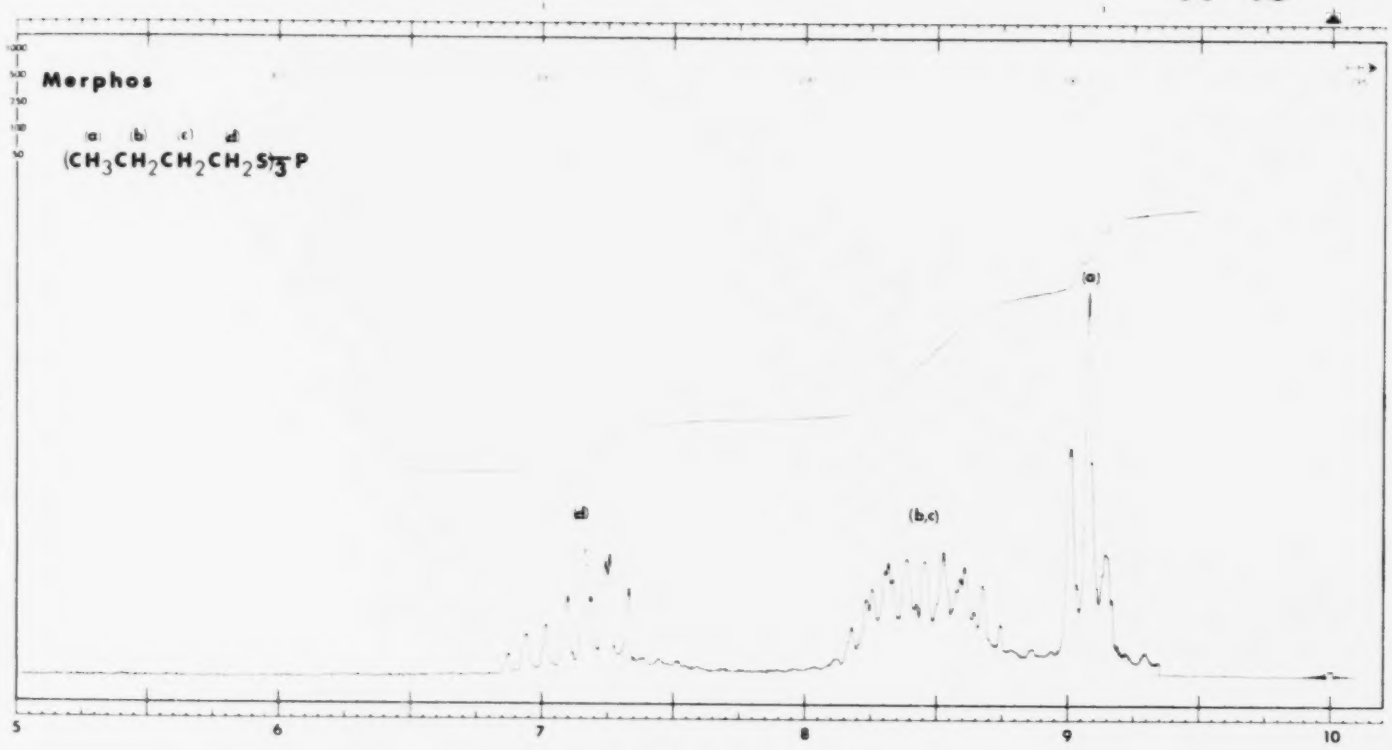


	T	J
a	9.03	7
b	8.27	7
c	5.88	9.5 (P-H)
		7 (H-H)

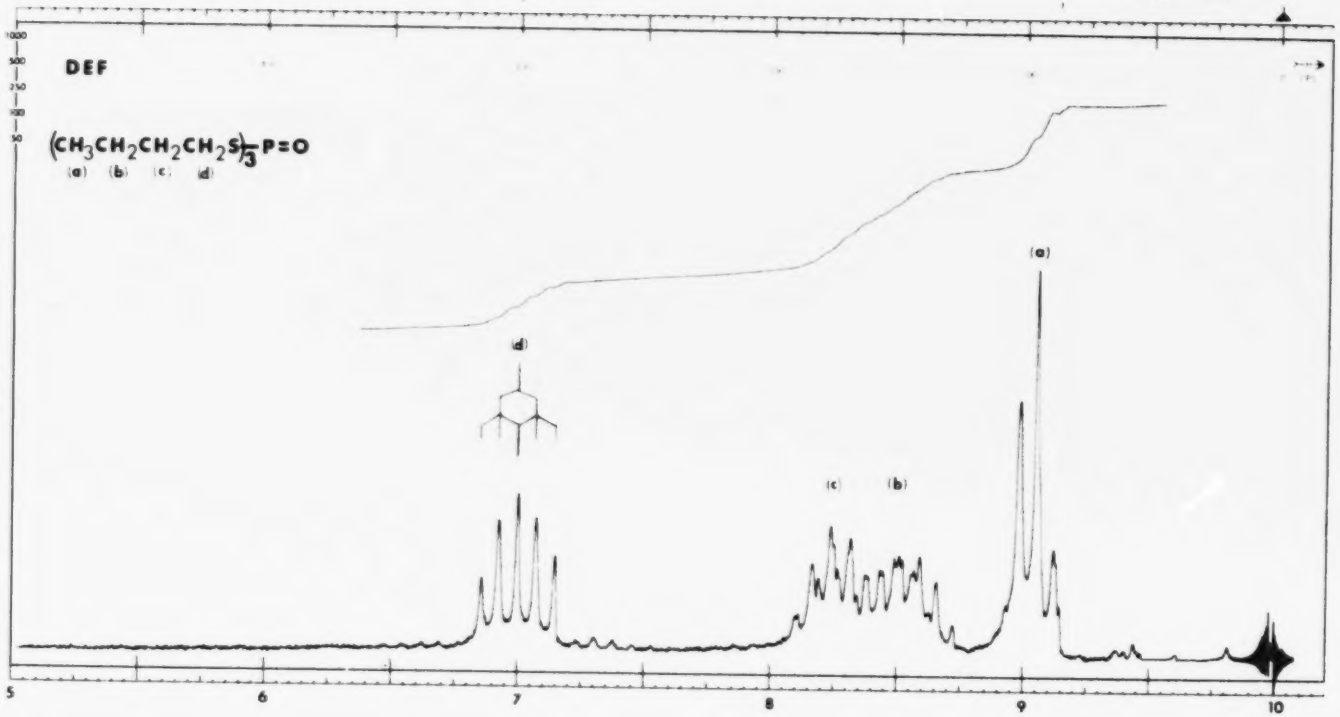


	T
a	5.4-6.7
b	2.6-3.4

A-48

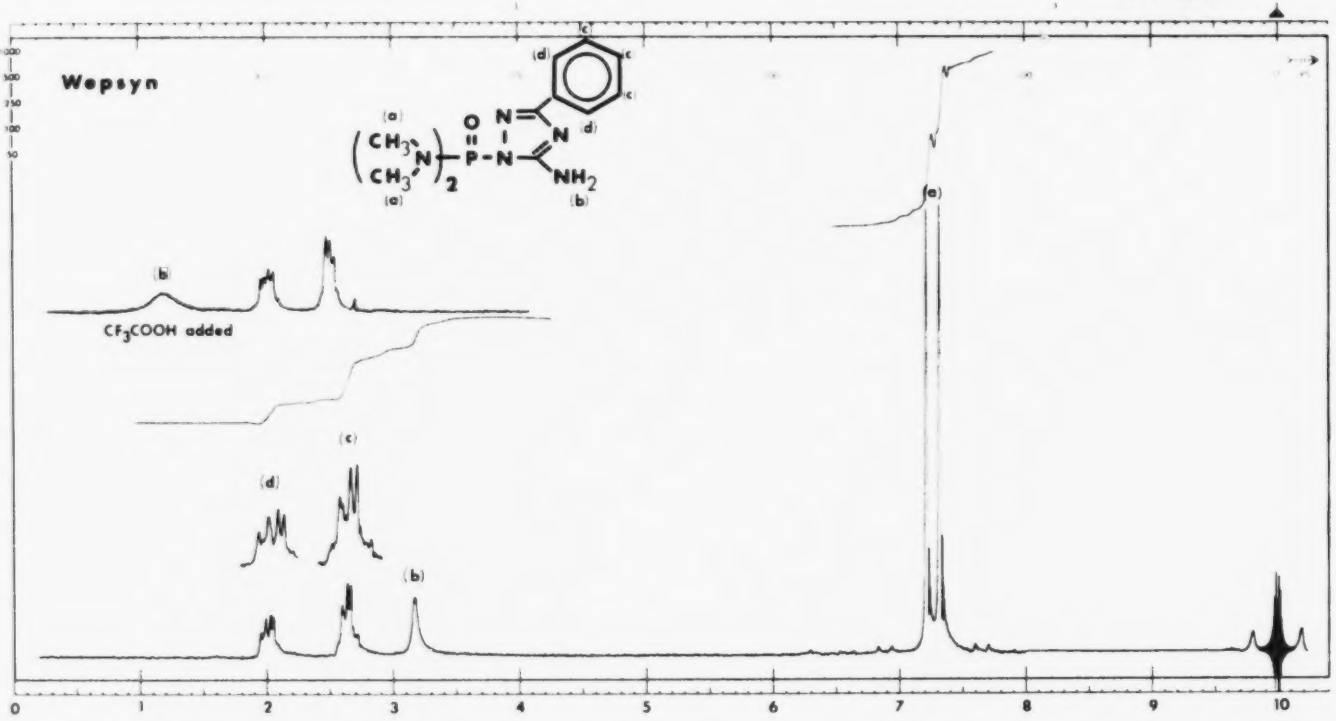


	T	J
a	9.08	7
b,c	8.1-8.8	
d	7.2	



	T	J
a	9.05	6.5
b	8.5	
c	8.25	
d	7.01	7(H-H) 15(P-H)

A-50



	T	J
a	7.24	10.5
b	3.14	
c	2.61	
d	1.98	

THE DDT-TYPE COMPOUNDS

Most DDT-type compounds contain para-disubstituted benzene rings whose protons produce complex multiplets. Each benzene ring contains four magnetically non-equivalent protons that form two pairs of equivalent nuclei with a chemical shift difference approximately equal to the coupling constants involved. This is defined as an AA'BB' system (6). The complex spectrum prevents interpretation by visual inspection, but an approximation of the ortho coupling constants and aromatic proton chemical shifts was obtained as described in a previous publication (4).

The ortho protons of compounds with the CCl_3 moiety on the α-carbon resonate at a significantly lower field (τ2.42-2.52) than ortho protons of compounds with other functional groups on the α-carbon (τ2.72-2.90). This large deshielding effect of the CCl_3 moiety may be explained by considering the molecular stereochemistry as observed in Leybold models. When three chlorines are substituted on the β-carbon, the ortho aromatic protons cannot escape the deshielding effect of the chlorine atoms. However, if only one chlorine atom is removed, the ortho protons are no longer forced into close proximity to the chlorine atoms. The deshielding effect of the CCl_3 group is greatest when chlorine substitution on one of the aromatic rings occurs in the ortho position. Examination of a Leybold model shows that a chlorine in the ortho position of a ring causes rotation of that ring around the aromatic-aliphatic C-C bond to be energetically unfavorable. The most favorable conformation places the remaining ortho proton near the β-carbon chlorines and the ortho chlorine as far as possible from the CCL_3 moiety.

The meta protons of the aromatic rings with para chlorine substituents resonate in a range from τ2.68-2.76. As expected, the benzylic

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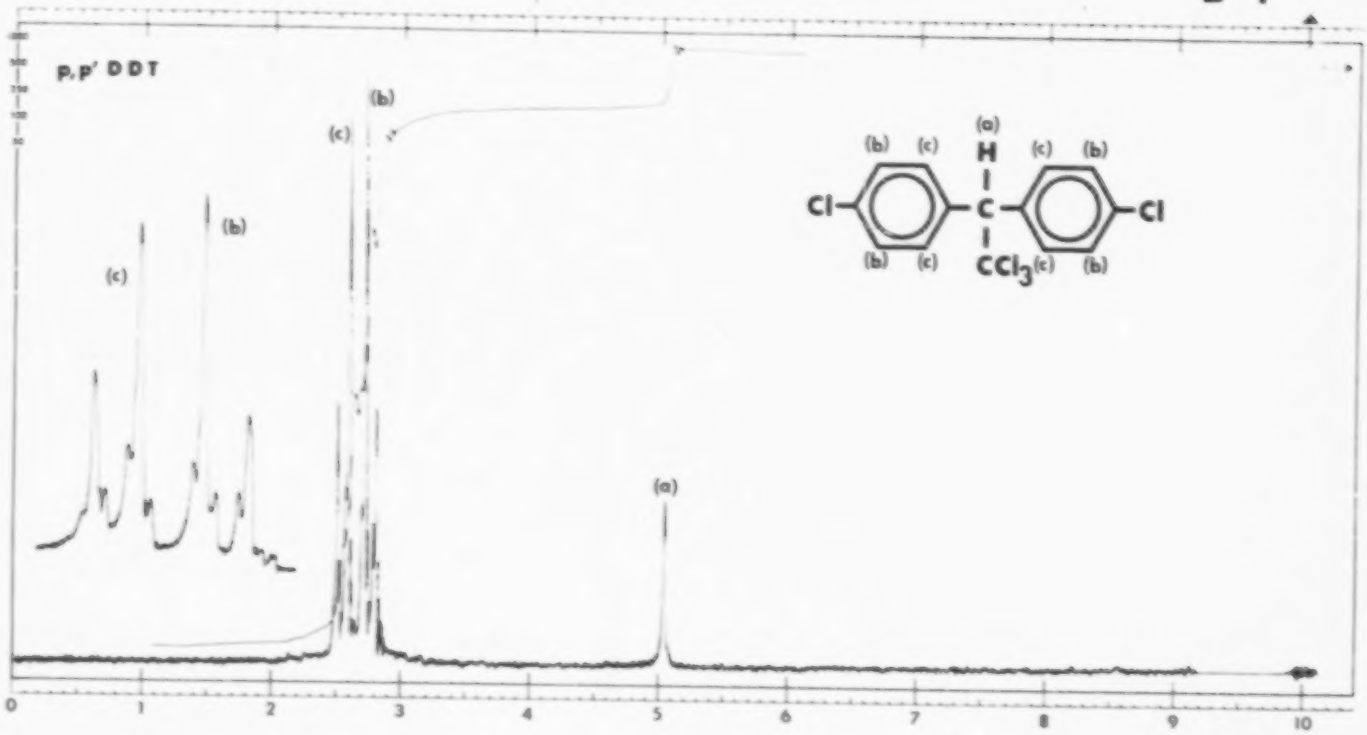
proton signals (τ5.06-6.0) are deshielded more by an ortho than a para chlorine on an aromatic ring.

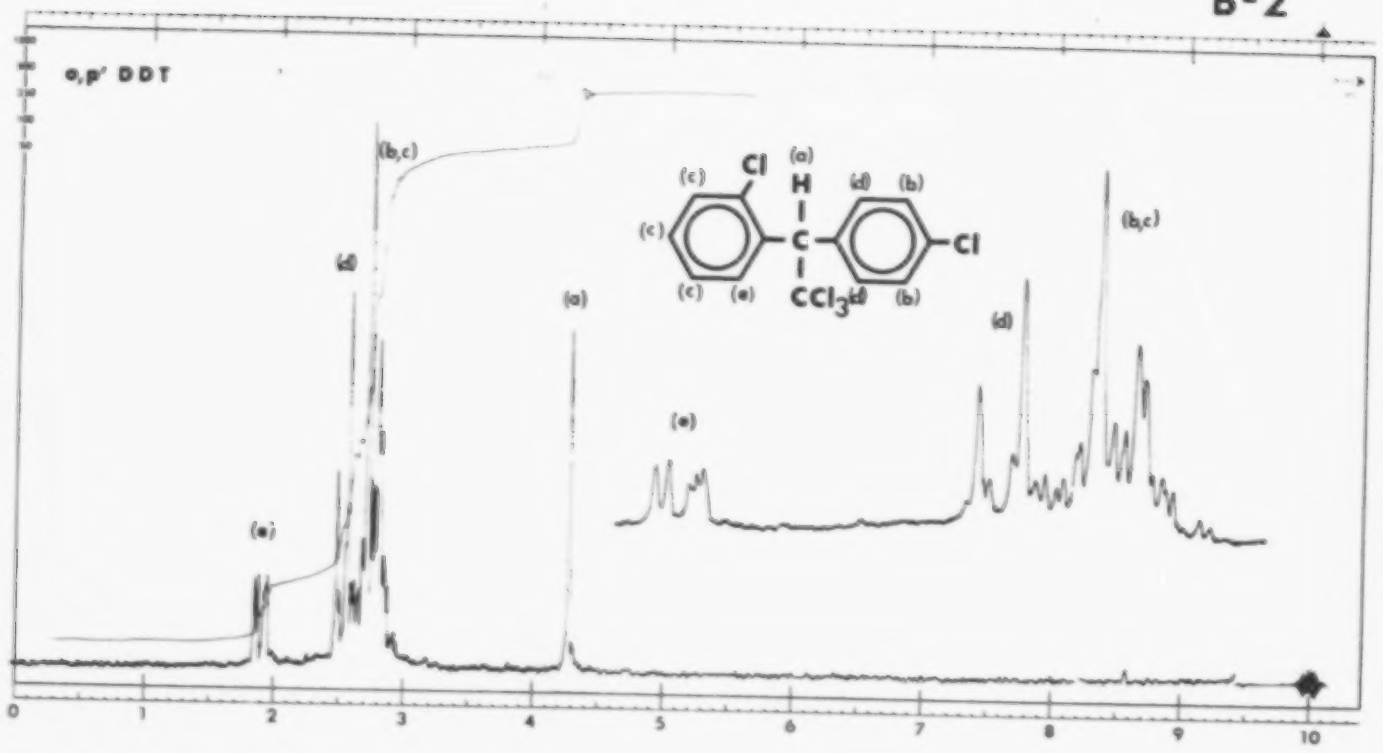
Technical DDT is a mixture of p,p'-DDT and o,p'-DDT. Peak area measurements by electronic integration of the part of the spectrum containing the signals of the benzylic protons (p,p'-DDT, τ5.00; o,p'-DDT, τ4.25) provide the isomeric composition of the sample (80% p,p'-DDT, 20% o,p'-DDT). The spectrum of Dilan, a mixture of Bulan and Prolan, contains only one benzylic peak but has two methyl signals with significantly different chemical shifts (triplet, τ9.11; doublet, τ8.54). The integration of these methyl signals provides the percentage of each compound in the mixture (62% Bulan, 38% Prolan).

B-1



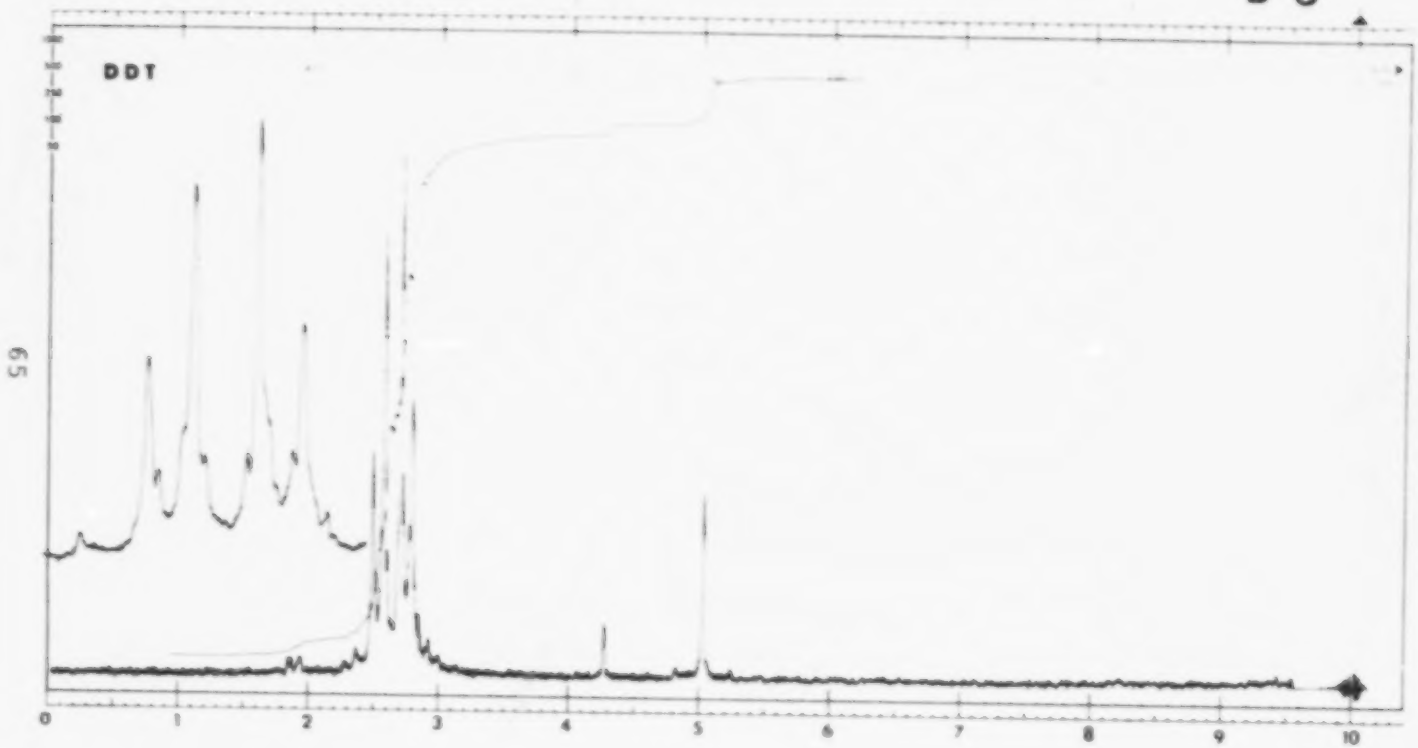
	T	J
a	5.00	
b	2.72	8.5
c	2.53	8.5

B-2



	T	J
a	4.25	
b	2.74	8.5
c	2.6-2.9	
d	2.52	8.5
e	1.88	

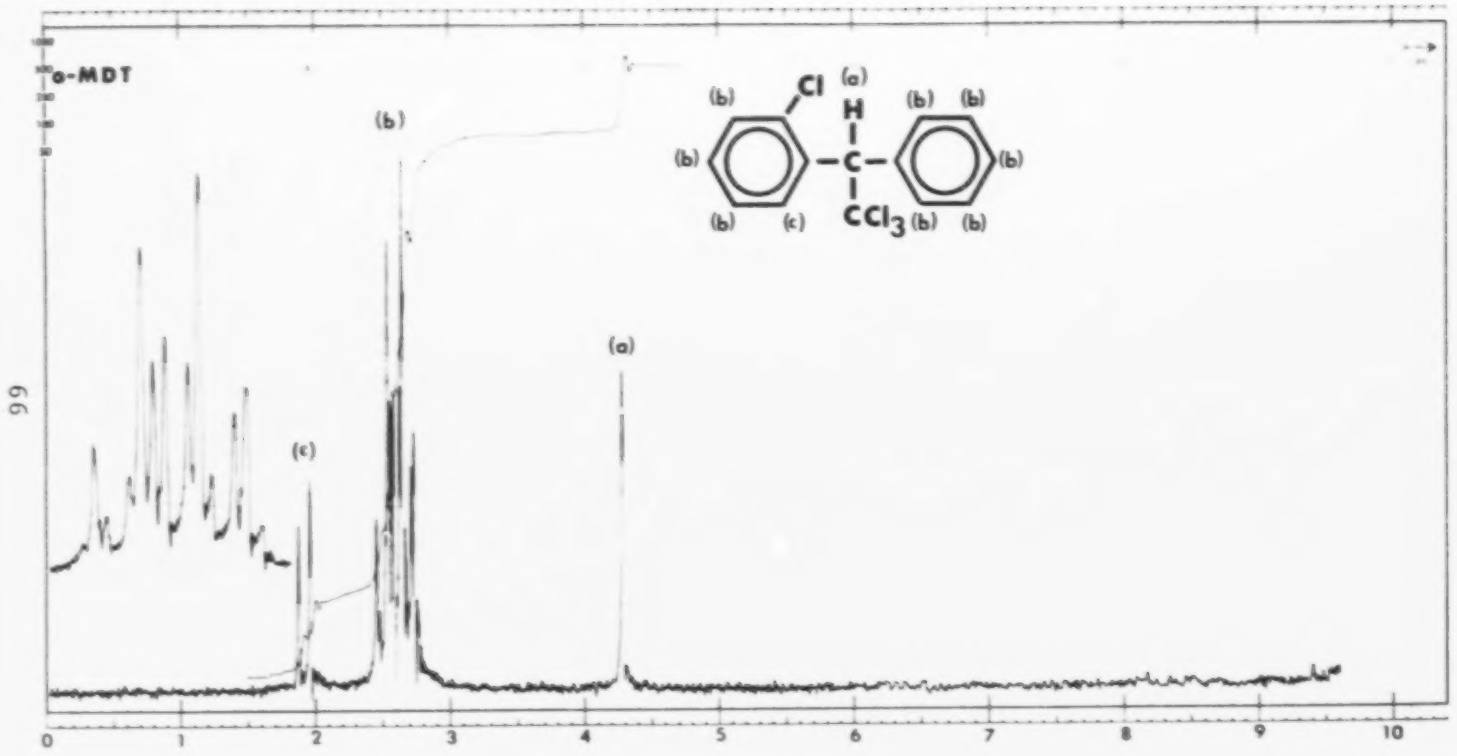
B-3



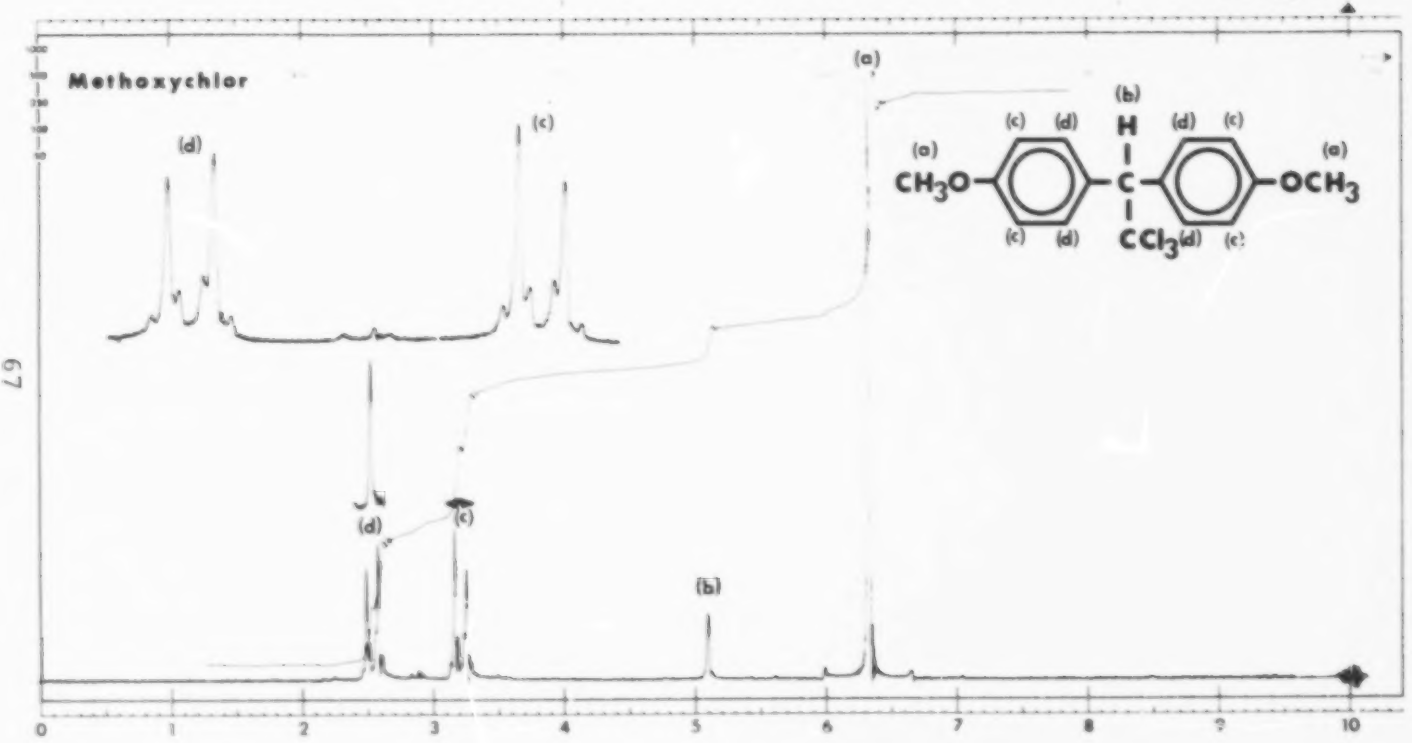
Technical DDT

Mixture of
o,p' DDT
and
p,p' DDT

B-4

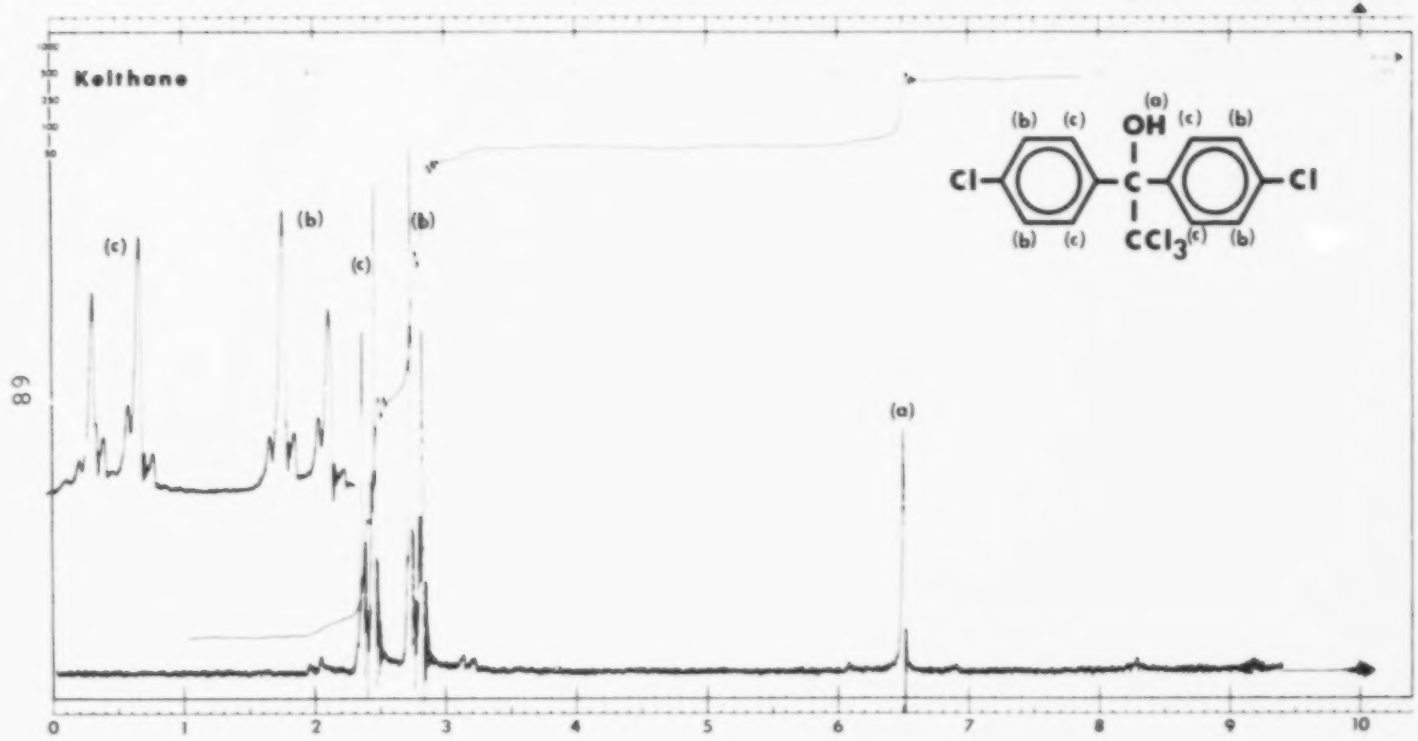


	T
a	4.28
b	2.4-2.8
c	1.84-1.98



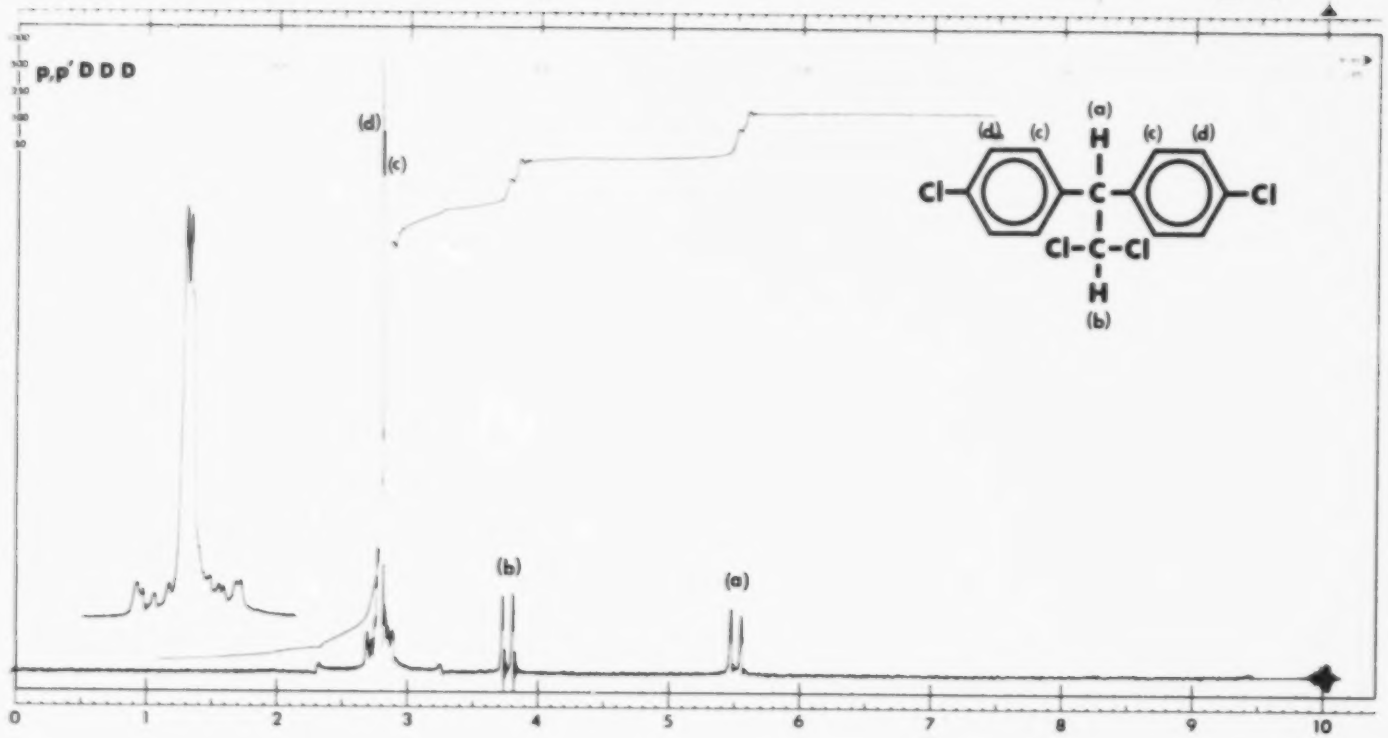
	T	J
a	6.29	
b	5.06	
c	3.18	9
d	2.52	9

B-6



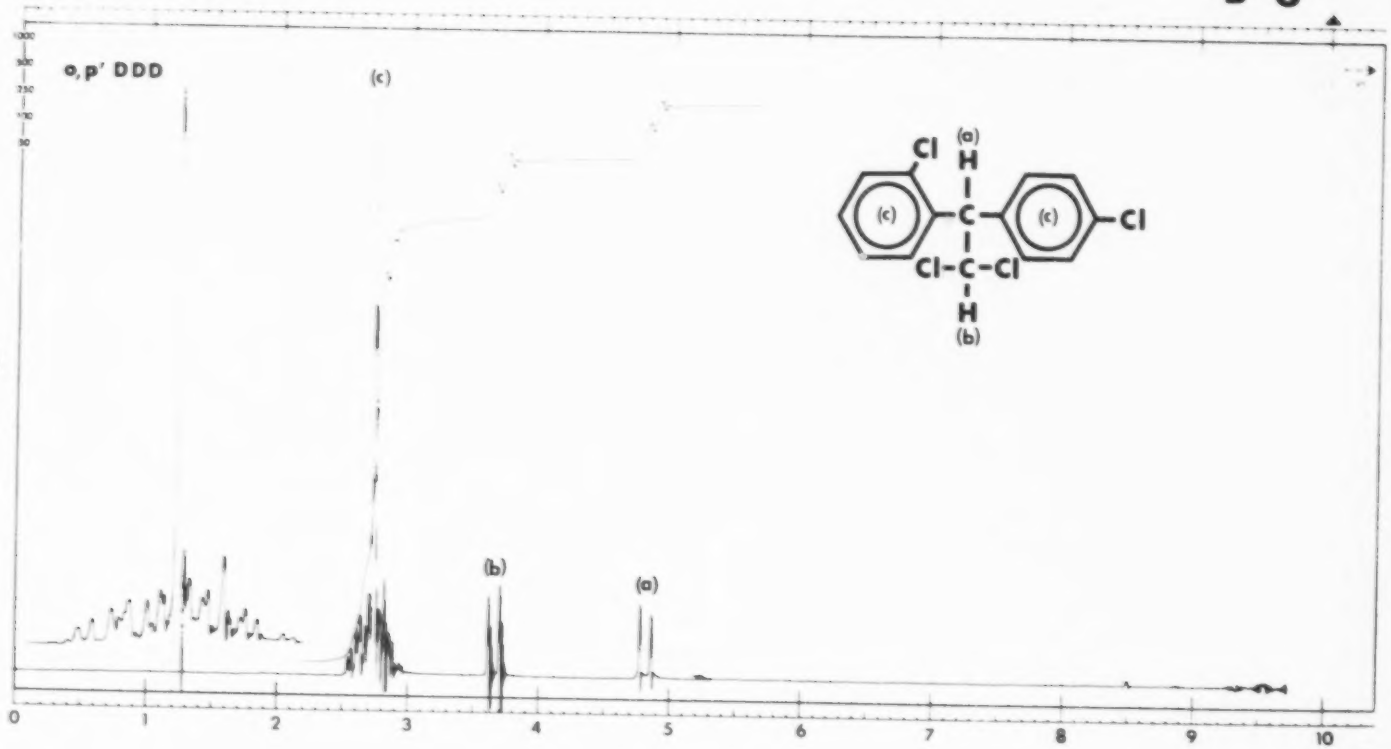
	T	J
a	6.48	
b	2.76	9
c	2.42	9

B-7



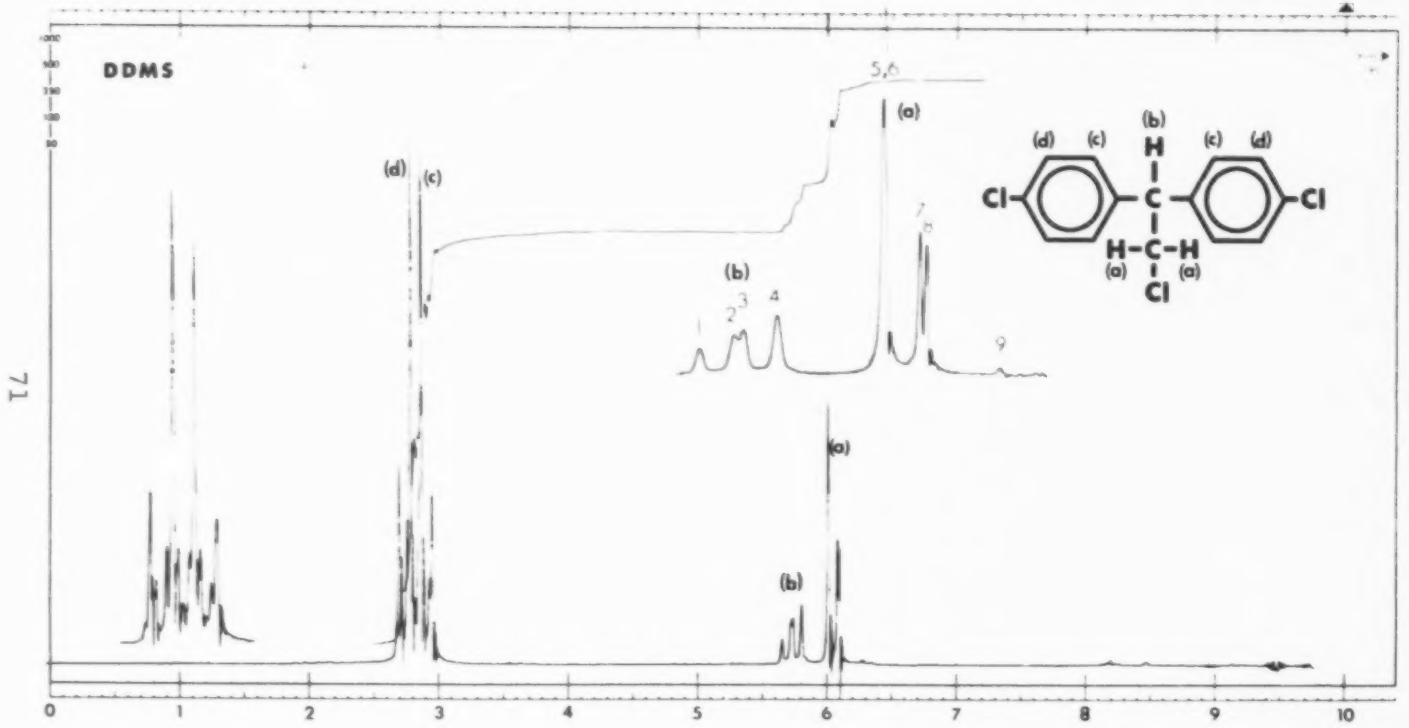
	T	J
a	5.49	8
b	3.74	8
c	2.78	9
d	2.74	9

B-8

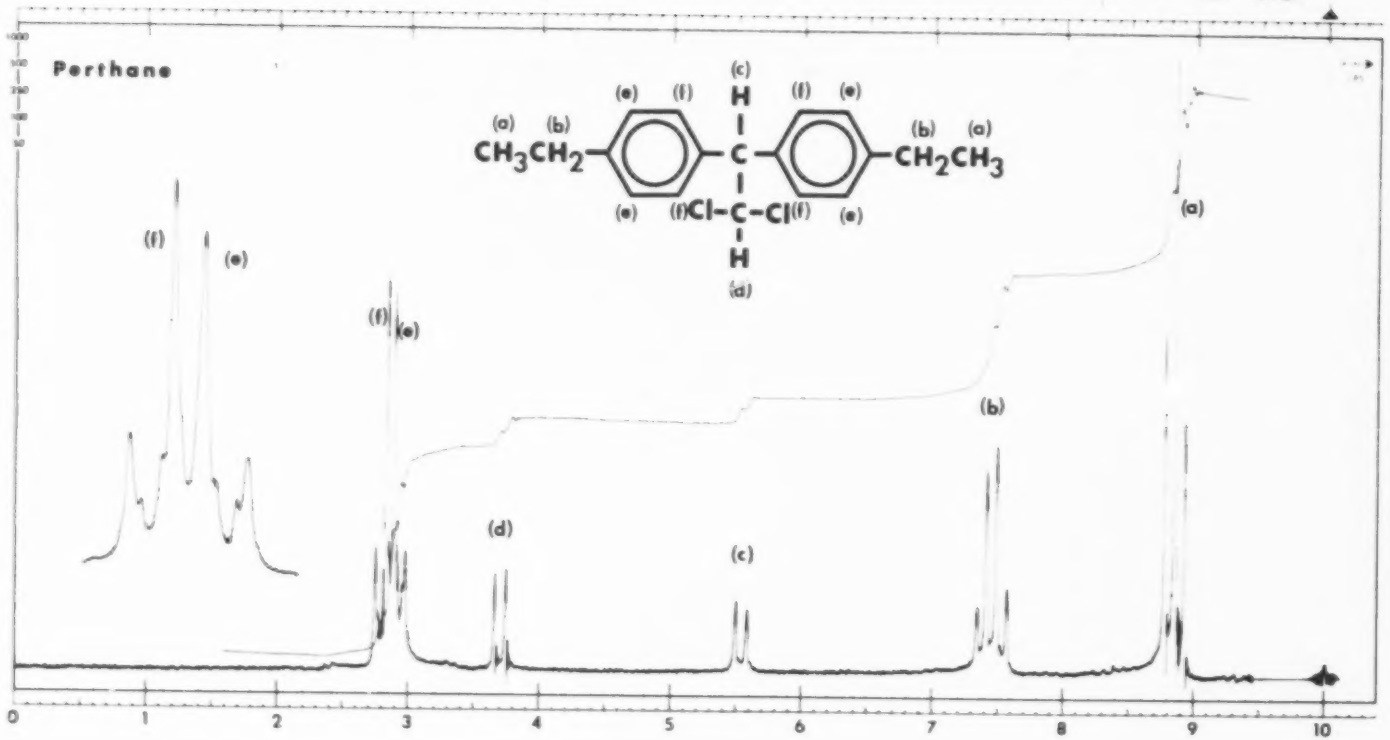


	T	J
a	4.82	8.5
b	3.64	8.5
c	2.5-2.9	

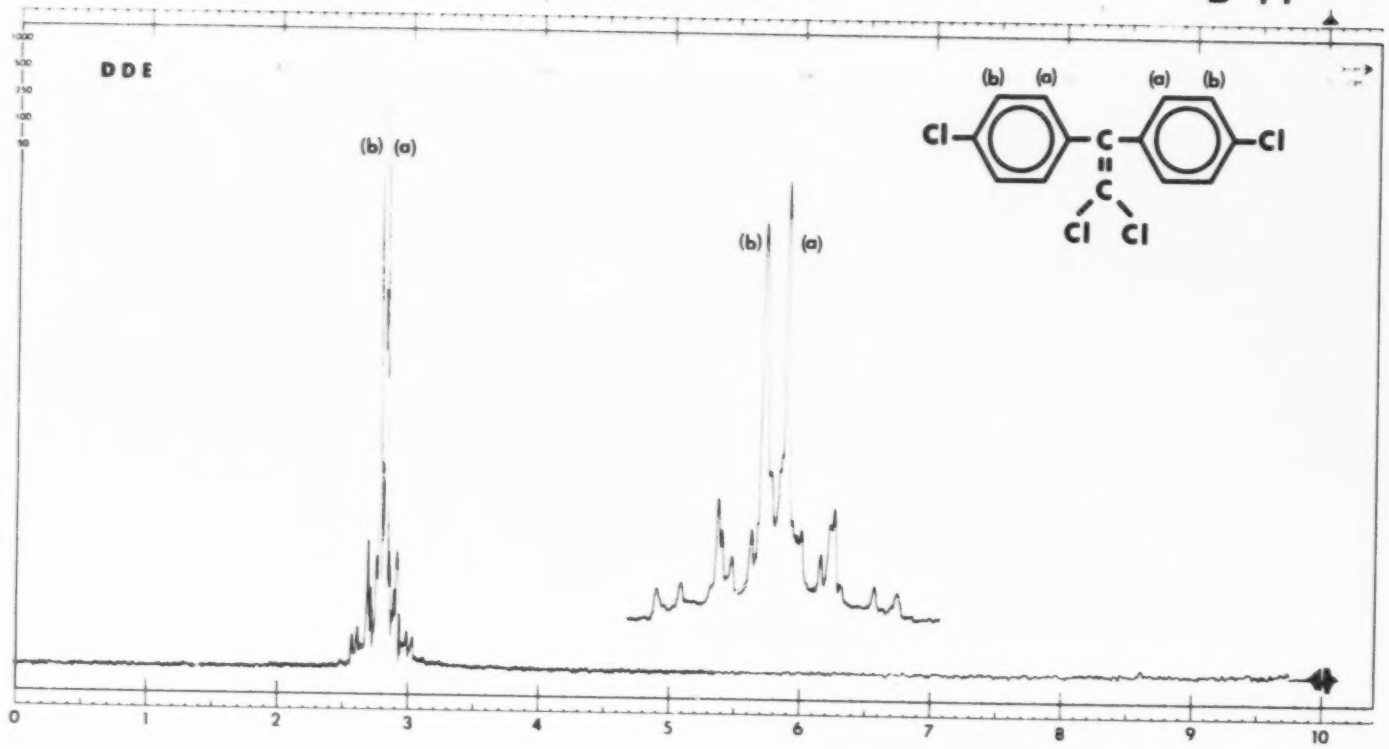
B-9



	T	J
a	6.05	8
b	5.75	8
c	2.88	8.5
d	2.74	8.5

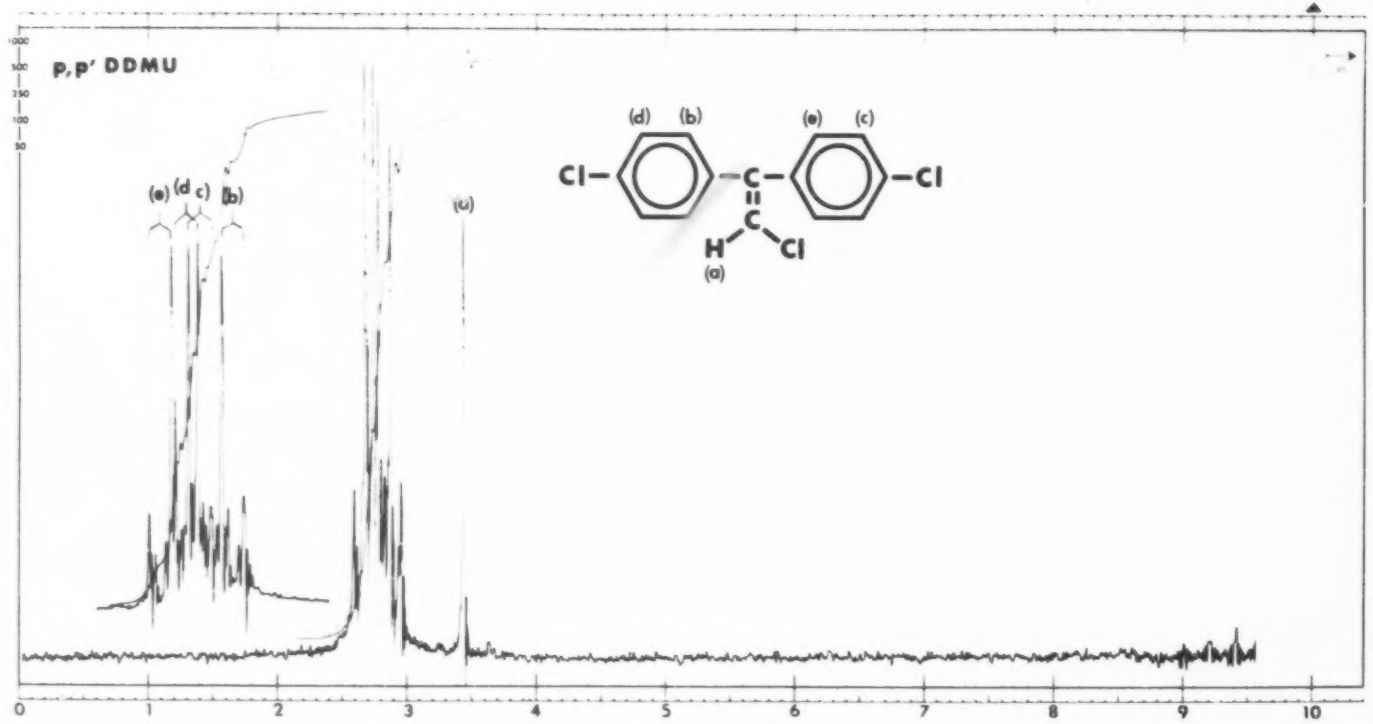


	T	J
a	8.84	7
b	7.43	7
c	5.50	8.5
d	3.68	8.5
e	2.92	9
f	2.80	9

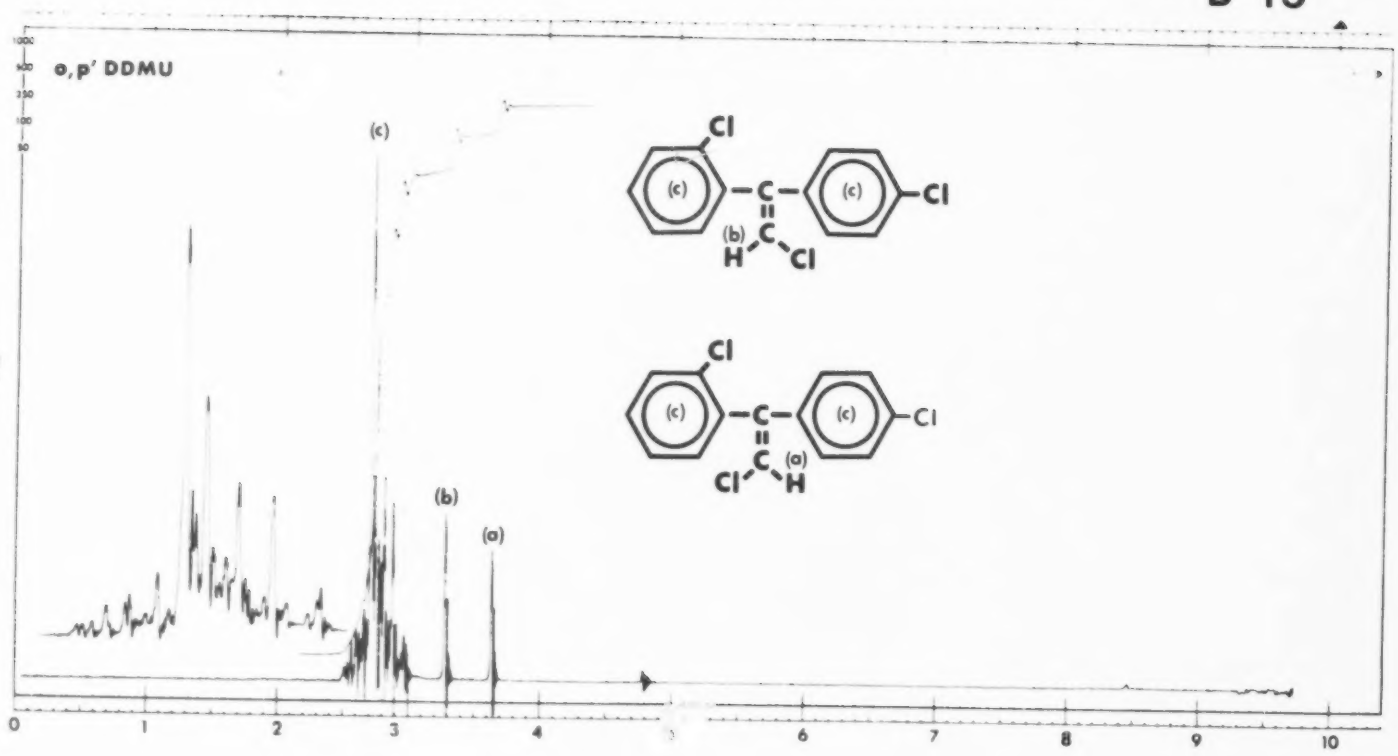


	T	J
a	2.88	9
b	2.75	9

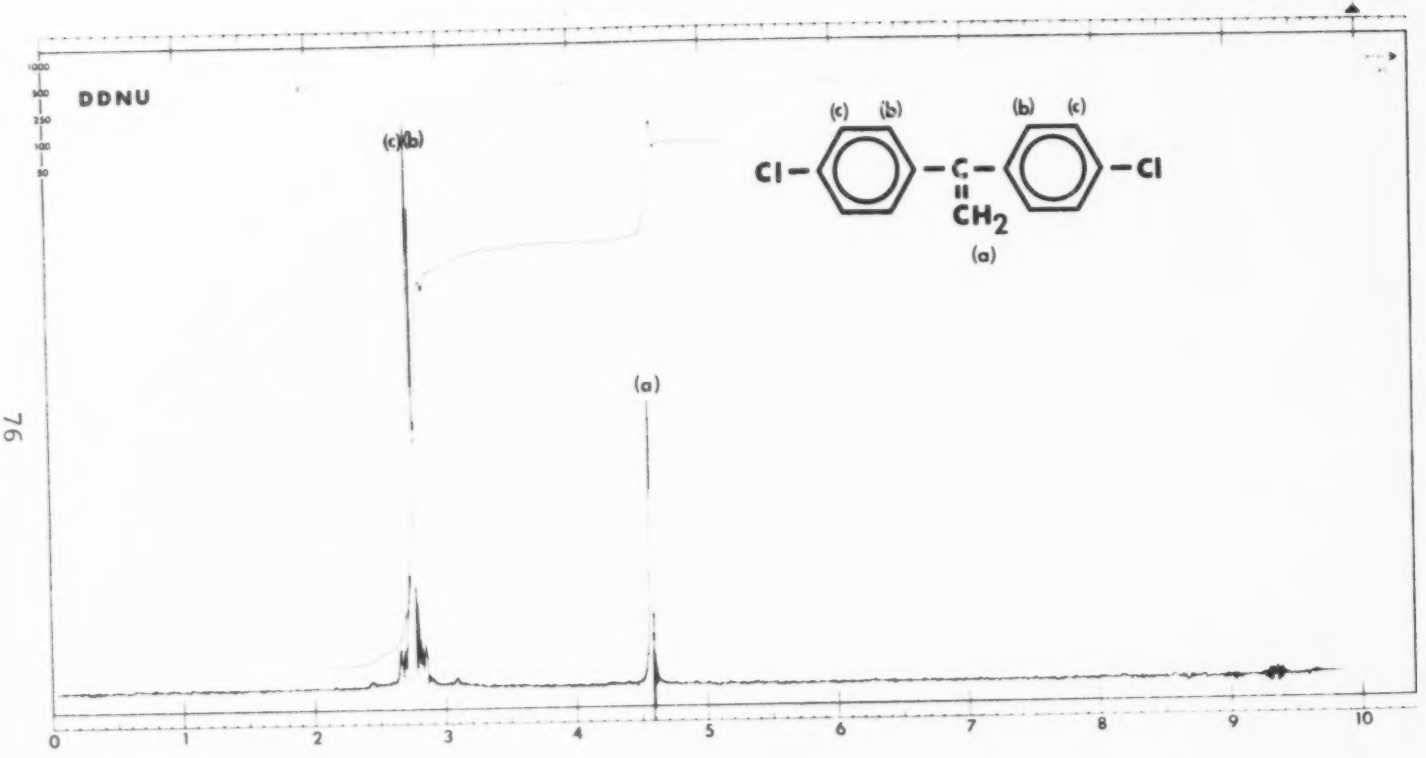
B-12



	T	J
a	3.45	
b	2.91	8.5
c	2.77	8.5
d	2.75	8.5
e	2.65	8.5

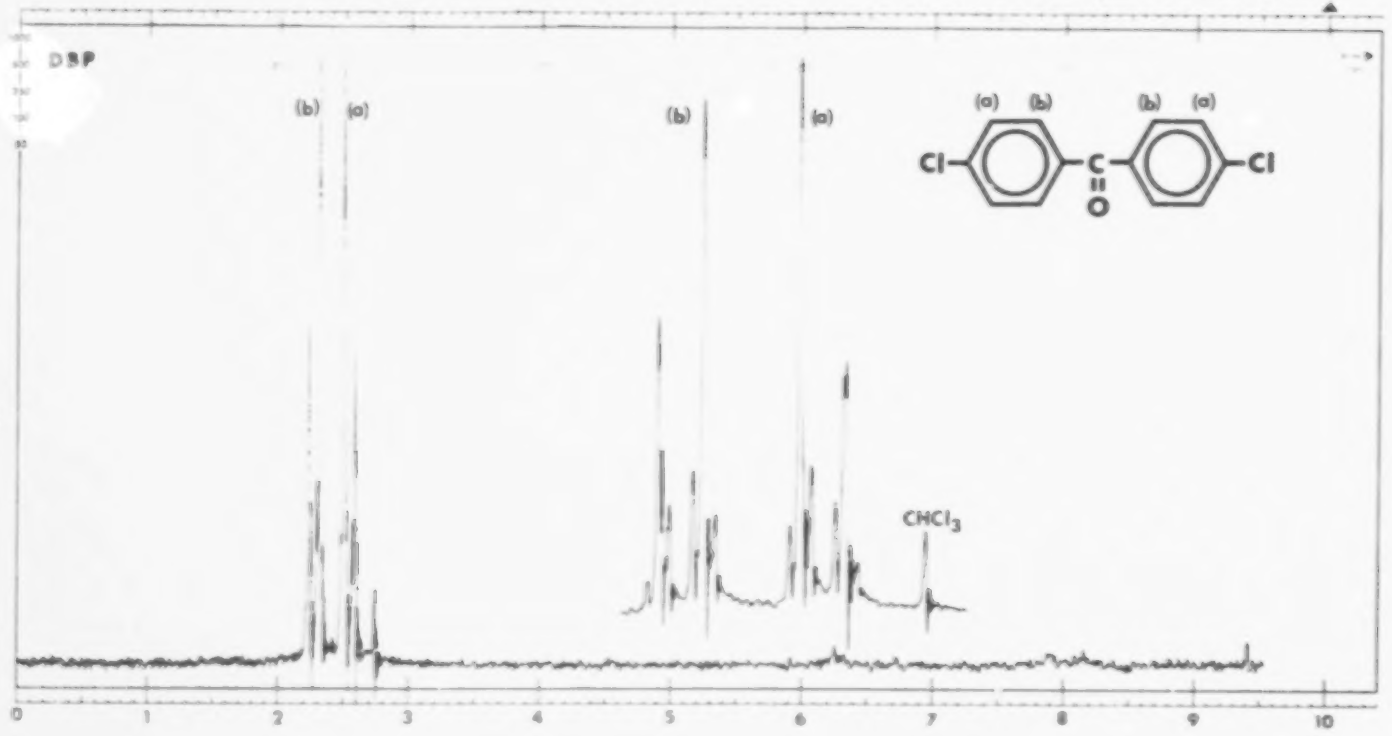


	τ
a	3.62
b	3.28
c	2.5-3.0



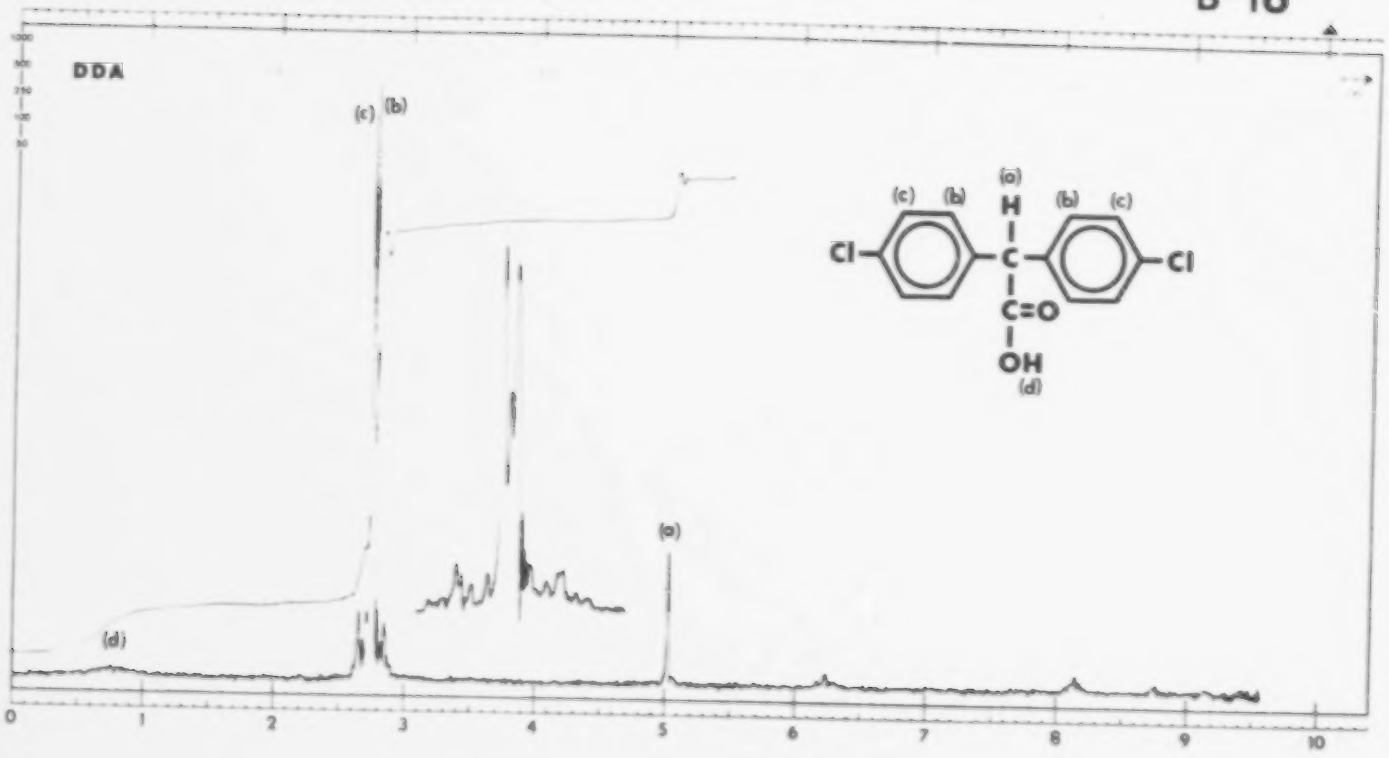
	T	J
a	4.59	
b	2.80	9
c	2.74	9

B-15

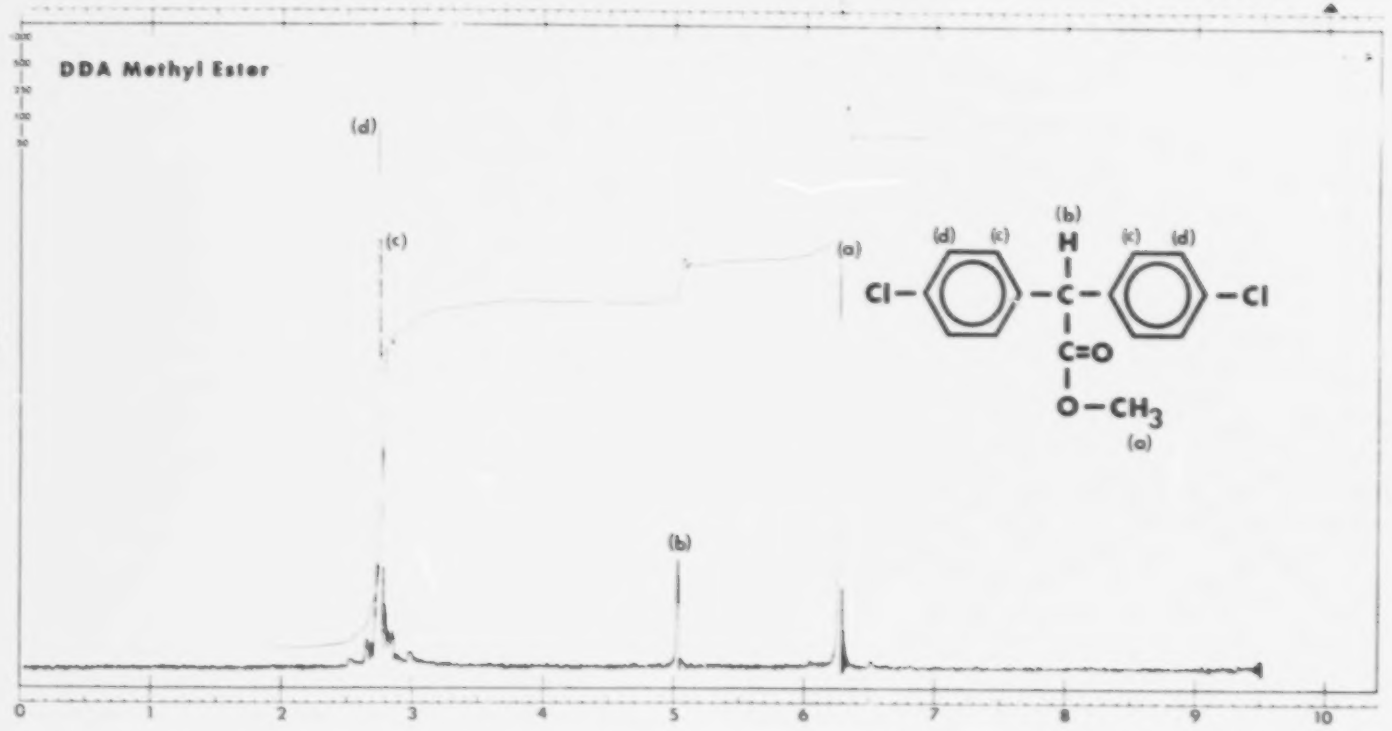


	T	J
a	2.55	8.5
b	2.29	8.5

B-16

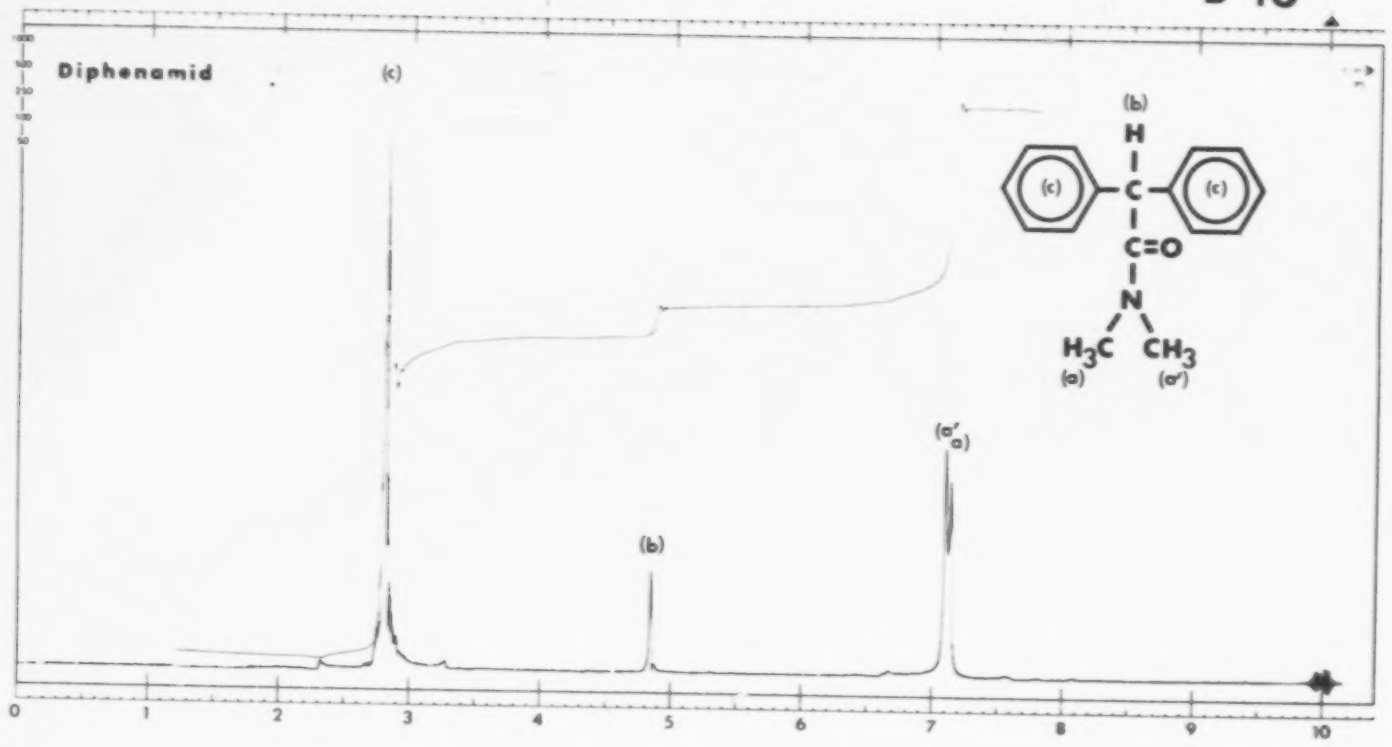


	T	J
a	5.03	
b	2.77	9
c	2.71	9
d	0.8	

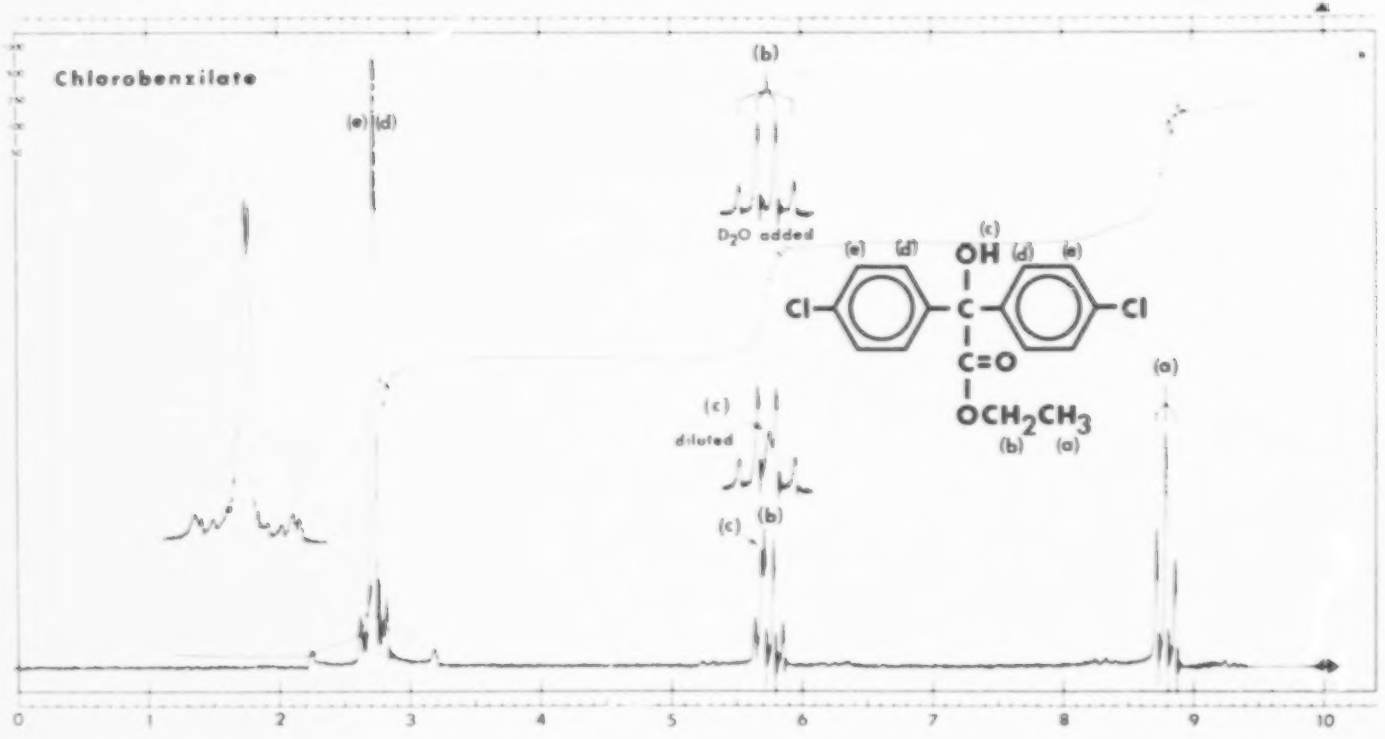


	T	J
a	6.29	
b	5.06	
c	2.79	9
d	2.73	9

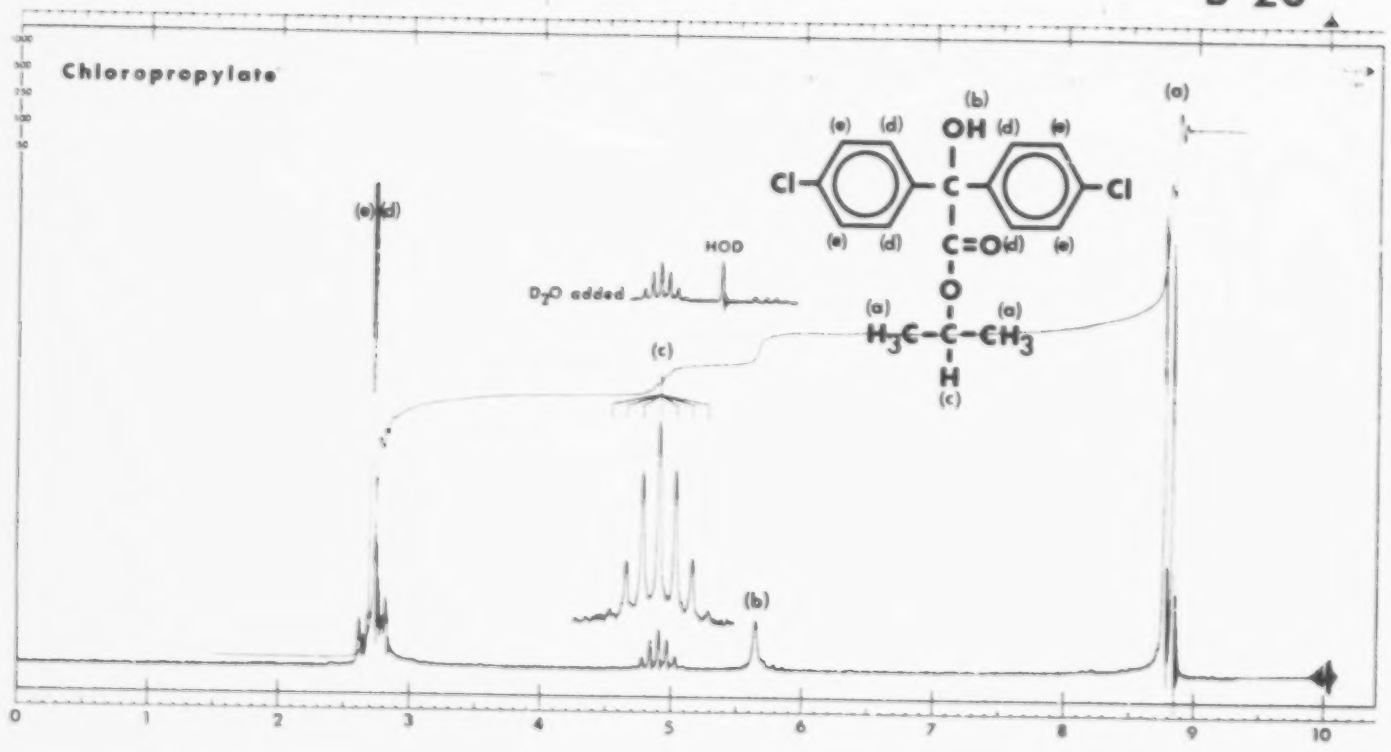
B-18



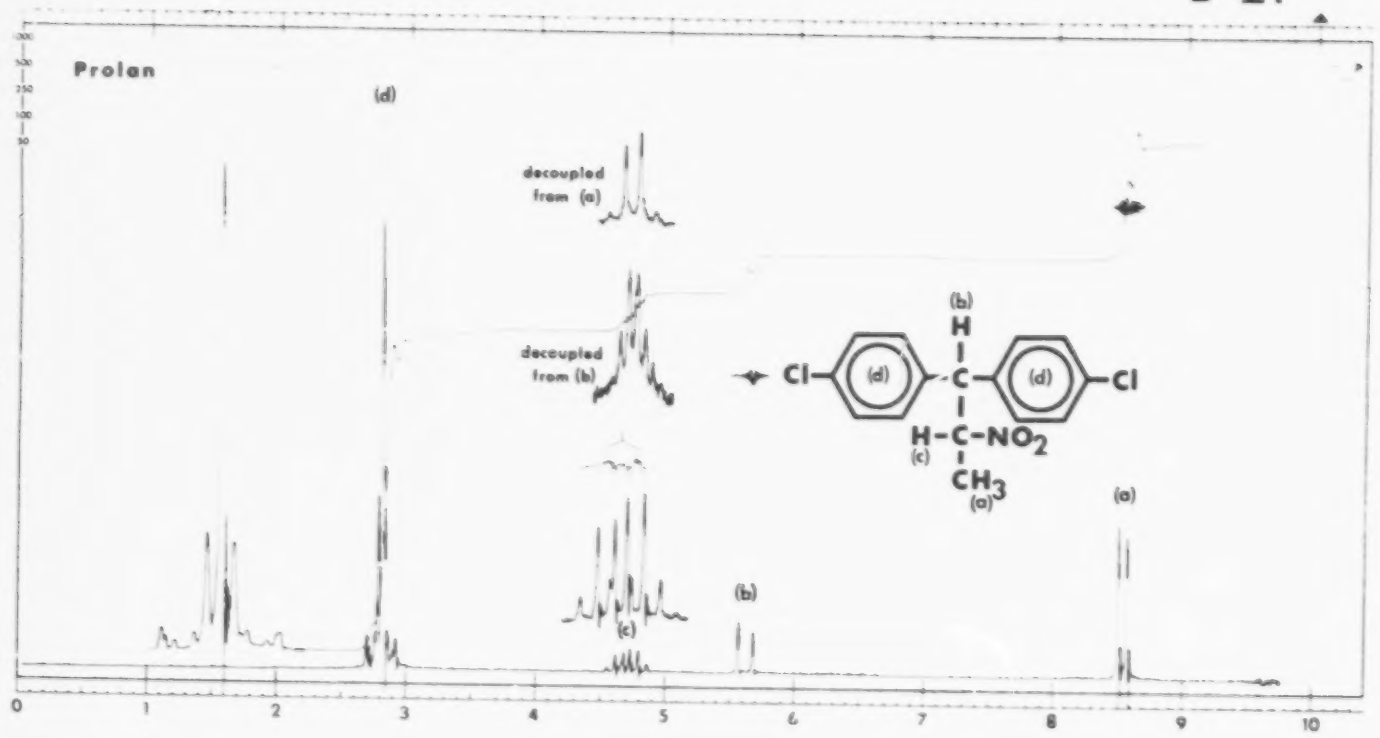
	T
a	7.12
a'	7.08
b	4.82
c	2.79



	T	J
a	8.78	7
b	5.73	7
c	5.68	
d	2.72	9
e	2.68	9

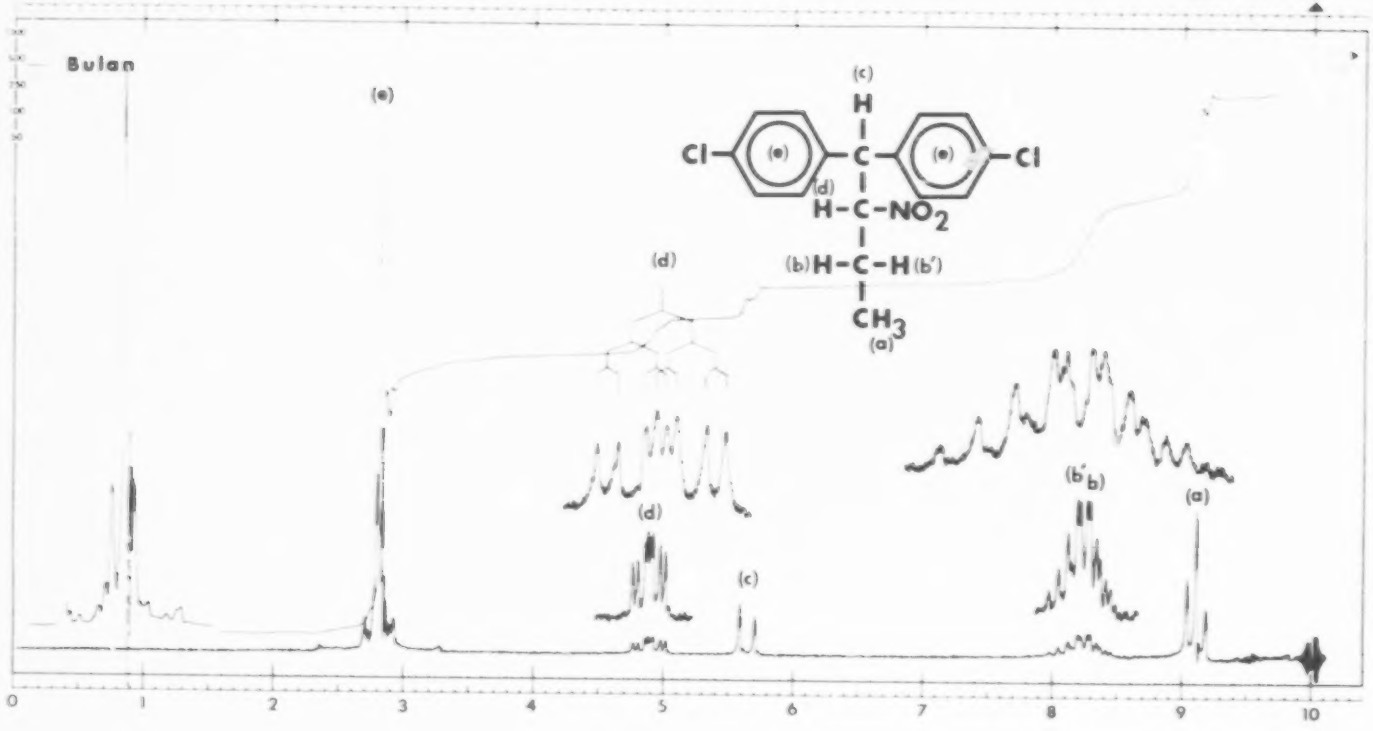


	T	J
a	8.79	6
b	5.63	
c	4.89	6
d	2.73	9
e	2.70	9



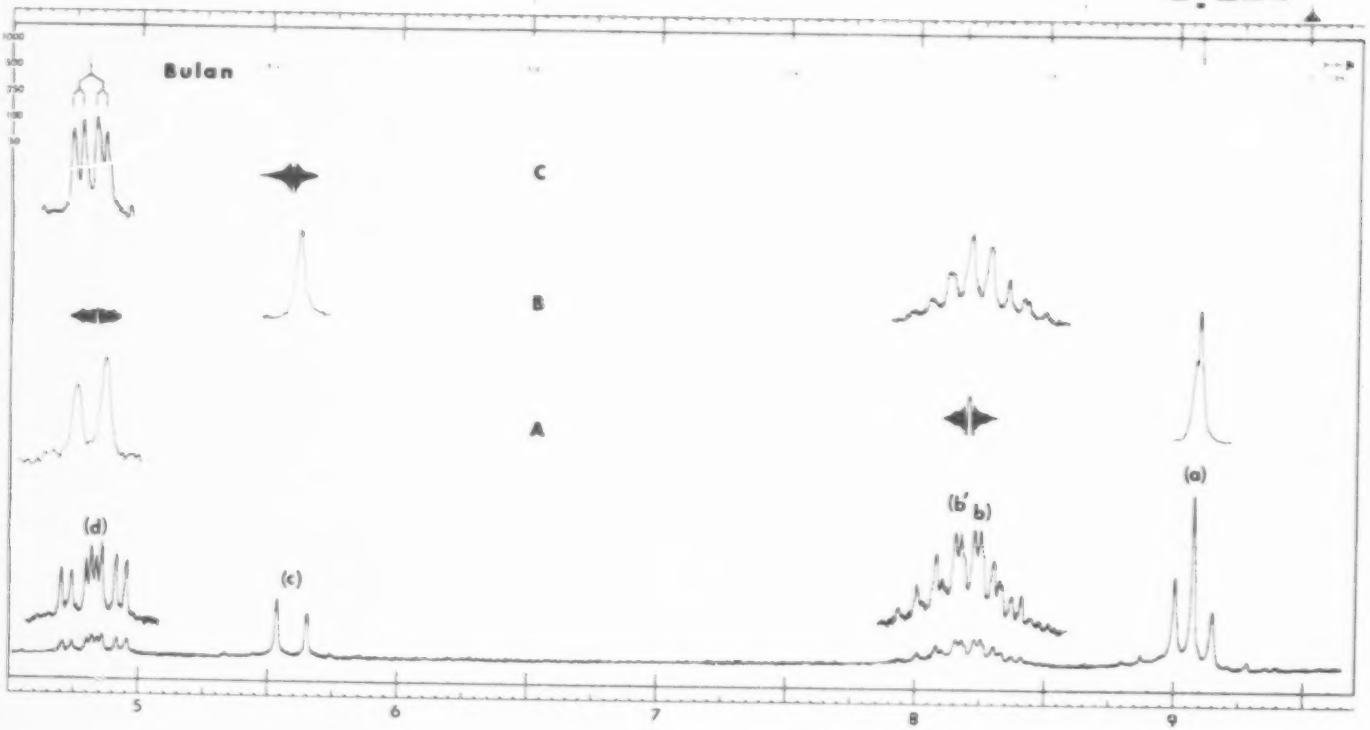
	T	J
a	8.54	6
b	5.62	12
c	4.70	$6(H_c\text{-}H_a)$ / $12(H_c\text{-}H_b)$
d	2.78	

B-22a



	T	J
a	9.11	7
b	8.23	
b'	8.25	
c	5.62	11.5
d	4.86	11.5(H_d-H_c)
		9.5(H_d-H_b)
		4 (H_d-H_b)
•	2.80	

B-22b



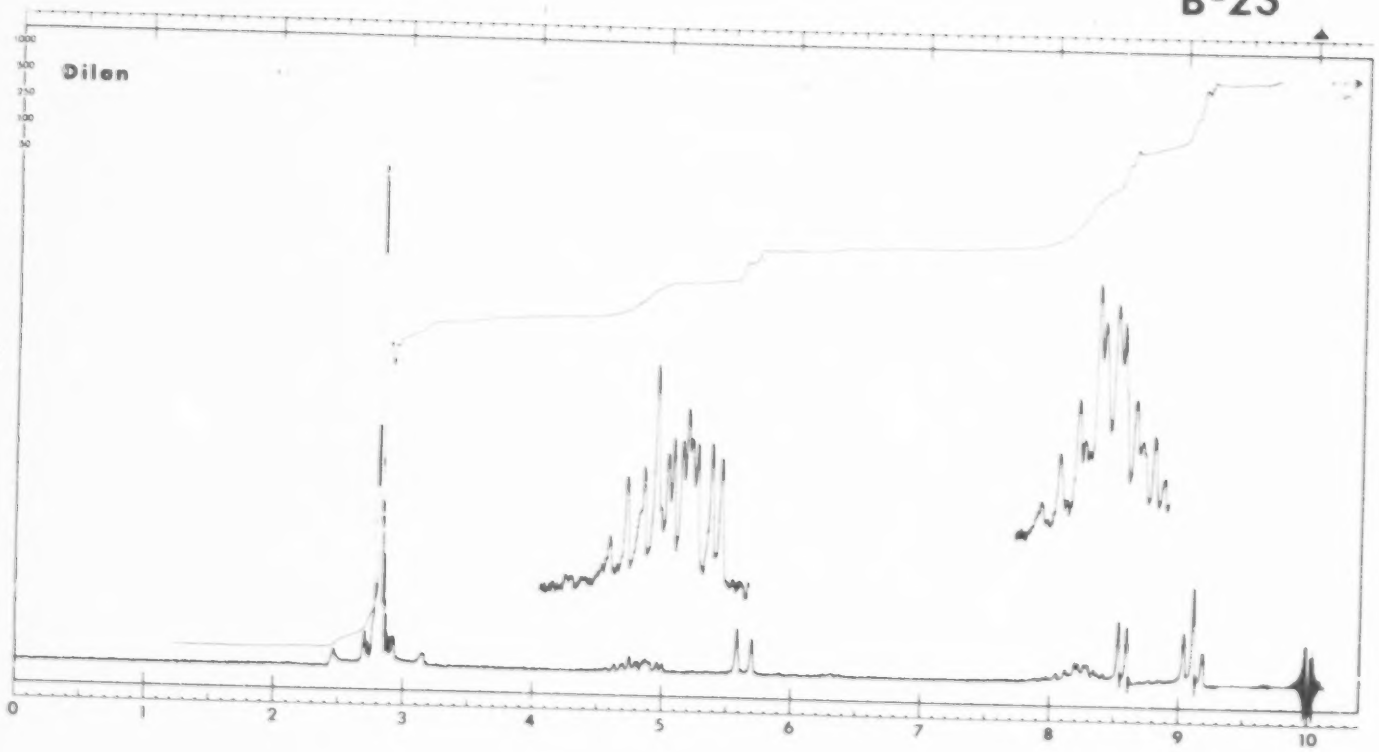
A H_a & H_d decoupled from H_b & $H_{b'}$

B H_c, H_b & $H_{b'}$ decoupled from H_d

C H_d decoupled from H_c

Sweep Width 500 cps

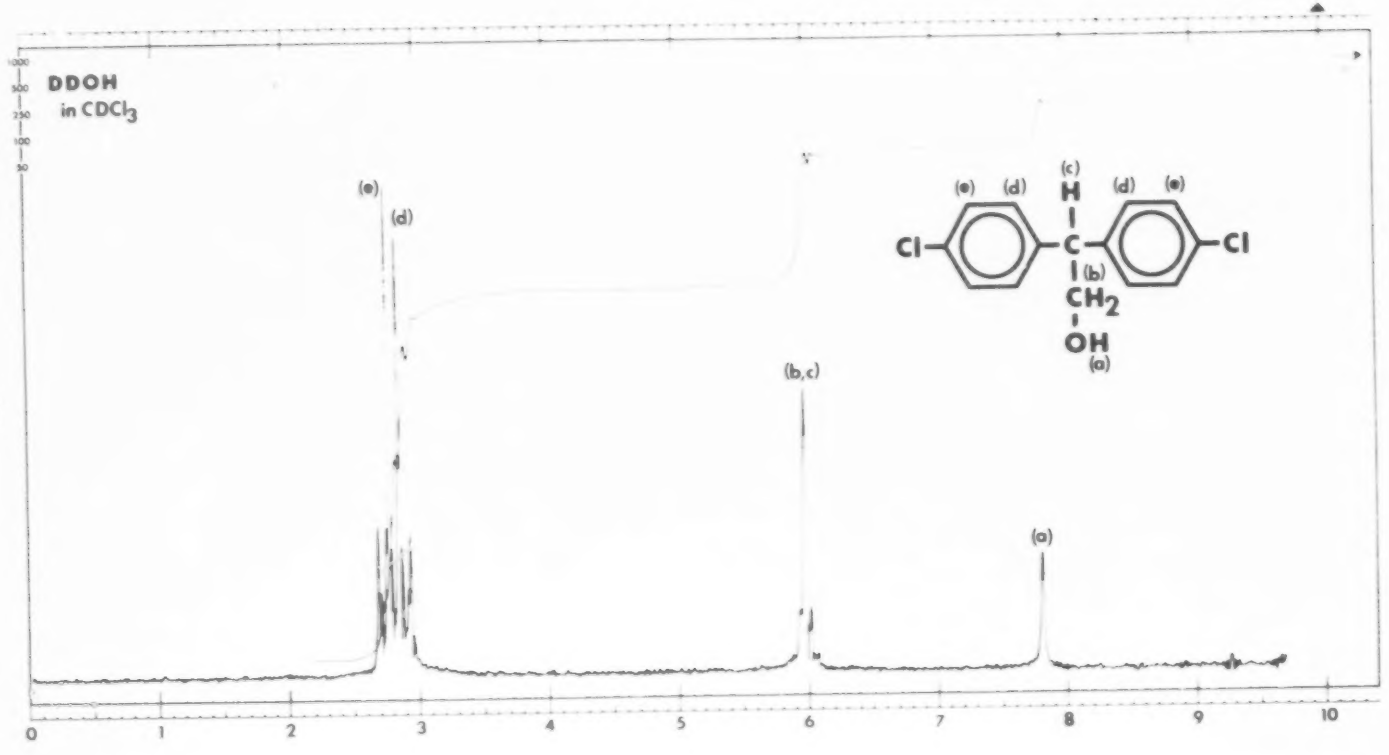
B-23



Mixture of

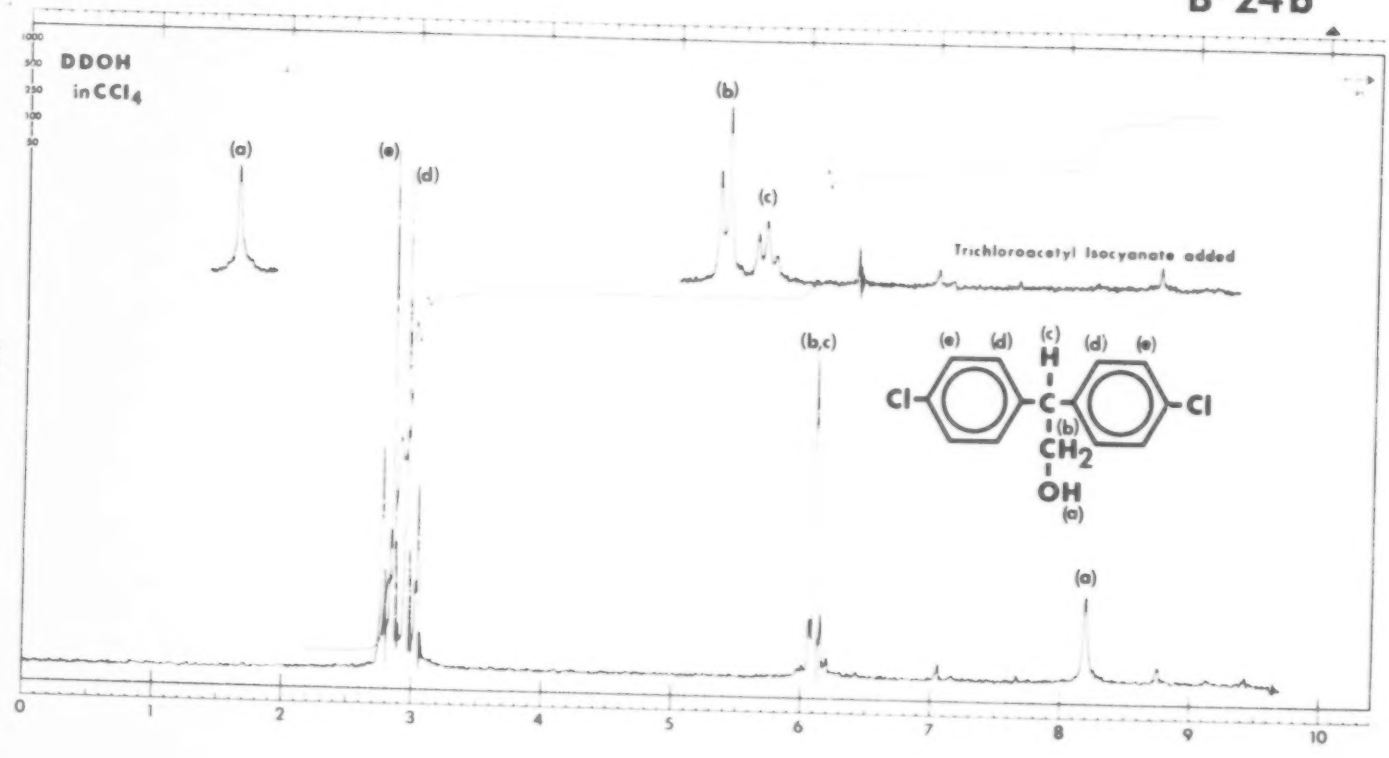
Prolan and Bulan

B-24a



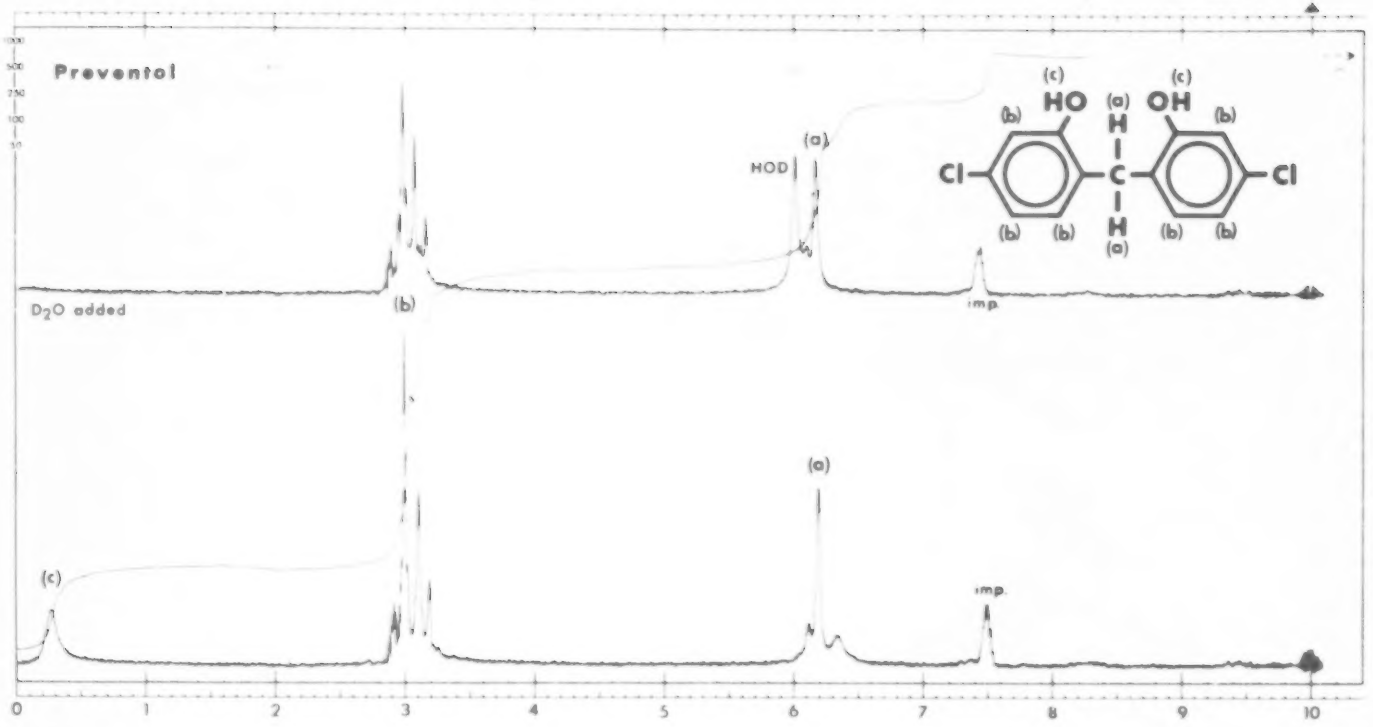
	T	J
a	7.82	
b,c	6.0	
d	2.90	9
e	2.75	9

B-24b



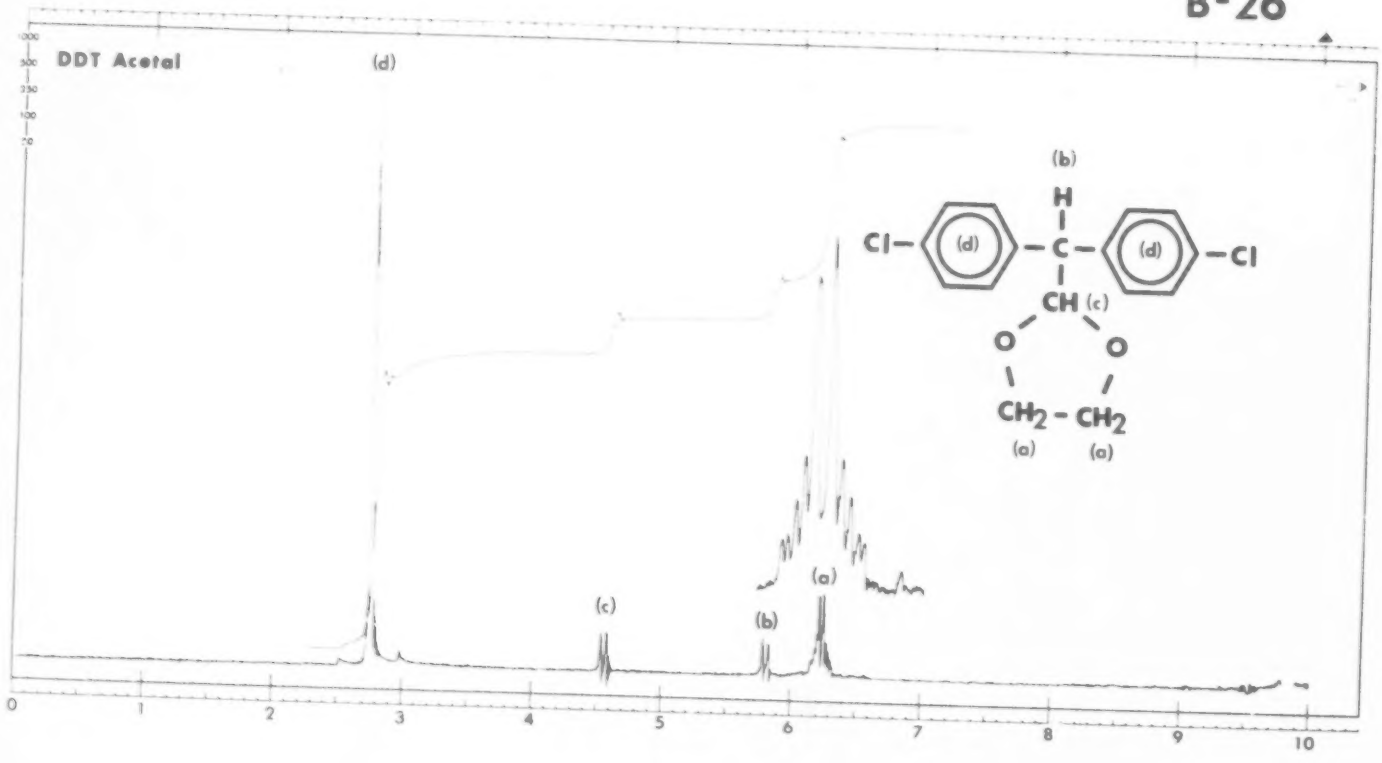
	T	J
a	8.19	
b,c	6.1	
d	2.97	9
e	2.81	9

B-25

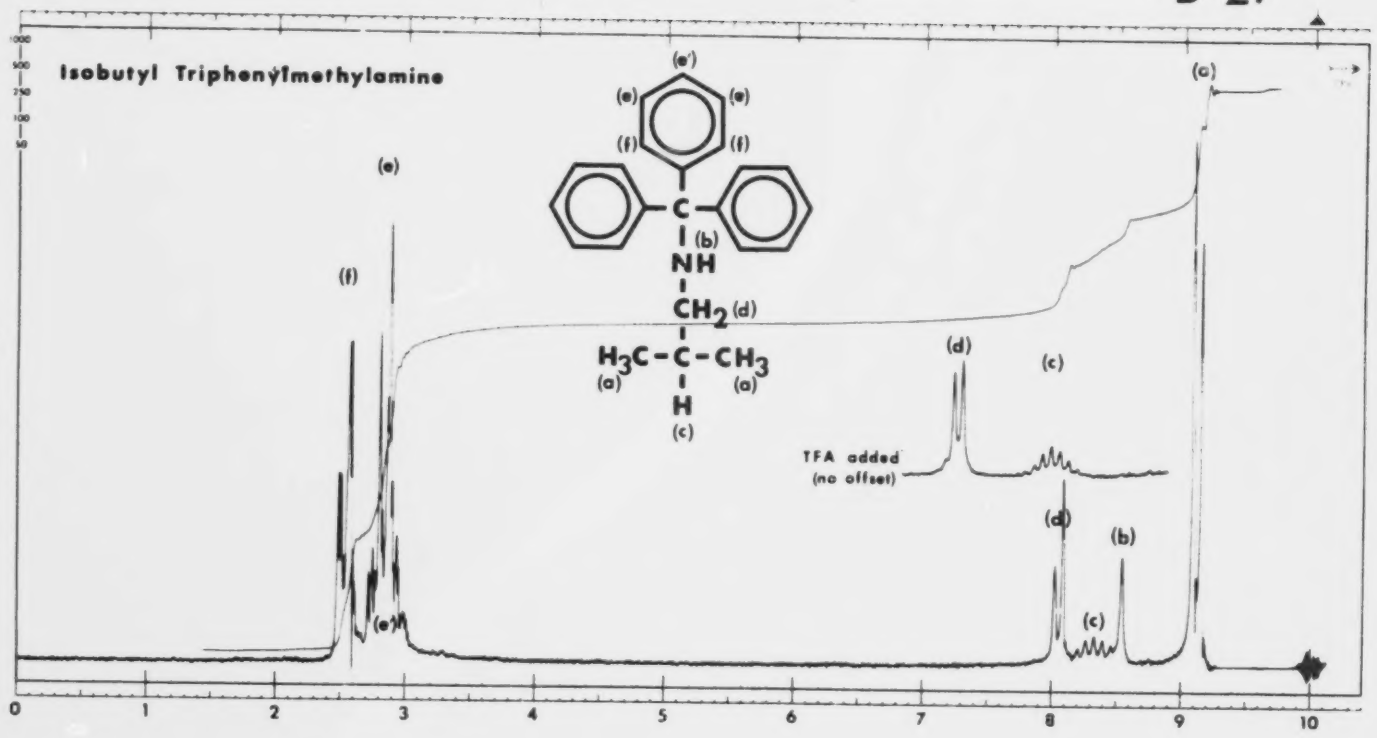


	T
a	6.17
b	2.9-3.1
c	0.3

B-26



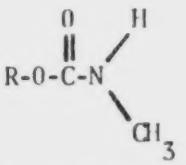
	T	J
a	6.24	
b	5.82	4
c	4.57	4
d	2.77	



	T	J
a	9.11	7
b	8.54	
c	8.33	
d	8.05	6
e,e'	2.7-3.0	
f	2.4-2.6	

THE CARBAMATE PESTICIDES

Thirteen carbamate pesticides included in this study have the general structure:



In all cases, the methyl protons resonate in a narrow range from τ7.20-7.29 and produce a doublet (J = 5 Hz) due to coupling of the methyl protons with the amide proton.

Although hindered rotation about the N-C=O bond of amides is quite common and produces both the cis and trans isomers, this phenomenon is observed at ambient temperature in only one of the N-monosubstituted carbamates, Azak. Other investigators (7,8) have also reported hindered rotation about the N-C=O bond in carbamates at low temperature but essentially free rotation at higher temperatures. In Azak, the bulky t-butyl groups substituted on the benzene ring in the ortho positions must sterically hinder rotation -- a signal is observed for each isomeric form at ambient temperature. Both N,N-dimethyl carbamates included in this study (Dimetilan and isolan) exhibit hindered rotation at ambient temperature and produce signals for both rotomer forms.

The chemical shifts of both the NH and NCH_3 proton signals of Zectran are dependent on solvent and concentration. Various concentrations of Zectran in three different solvents were used to study the effects of solute-solute and solute-solvent association (5).

The signals of the protons near or adjacent to nitrogen in many of these compounds show broadening due to the quadrupole moment of the nitrogen

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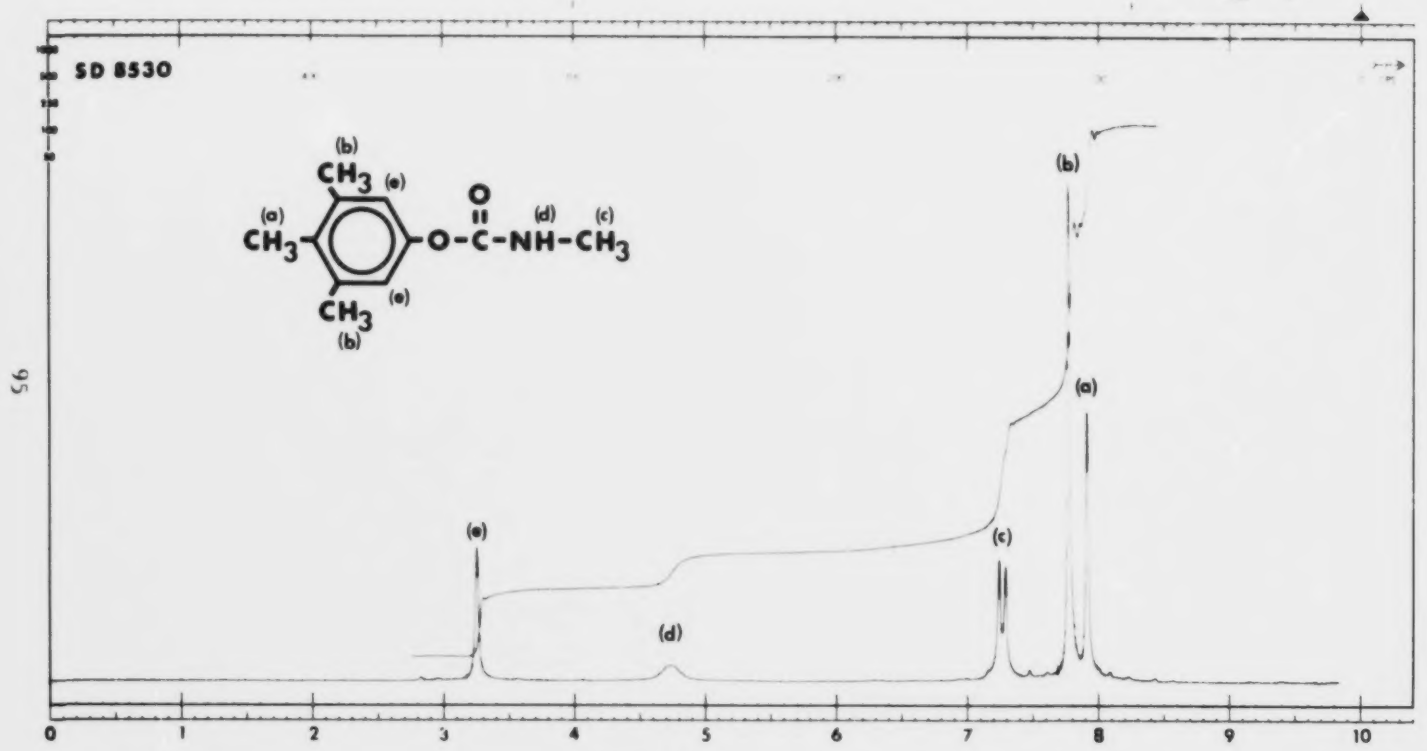
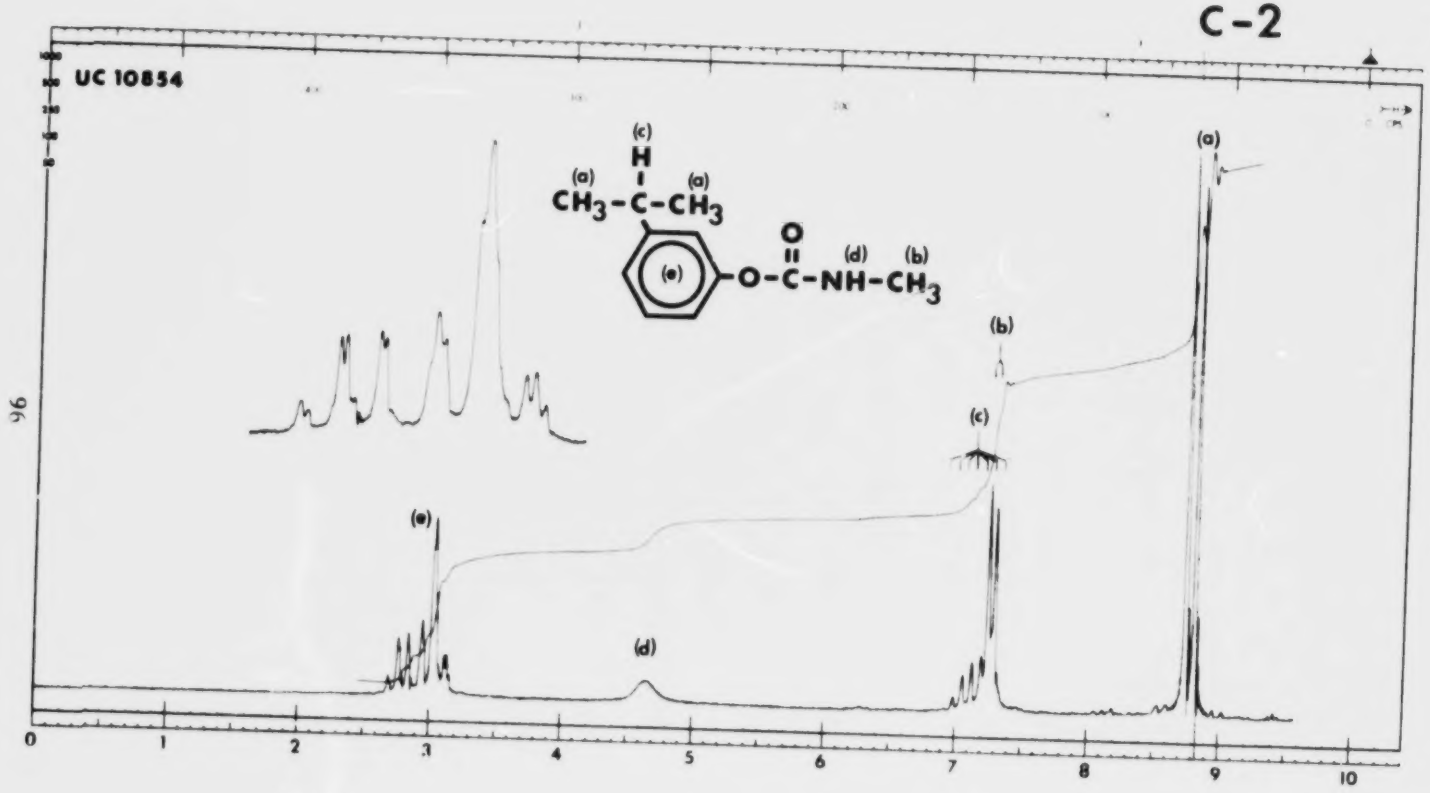
nucleus as well as some hindrance to rotation (7, 9). Increasing the sample temperature sharpens peaks that are broadened due to one or both effects (10, 11). Low temperature studies (5) confirmed that rotation is hindered in both the thiolcarbamates (example: sutan) and the dithiocarbamates (example: Vegadex).

C-1



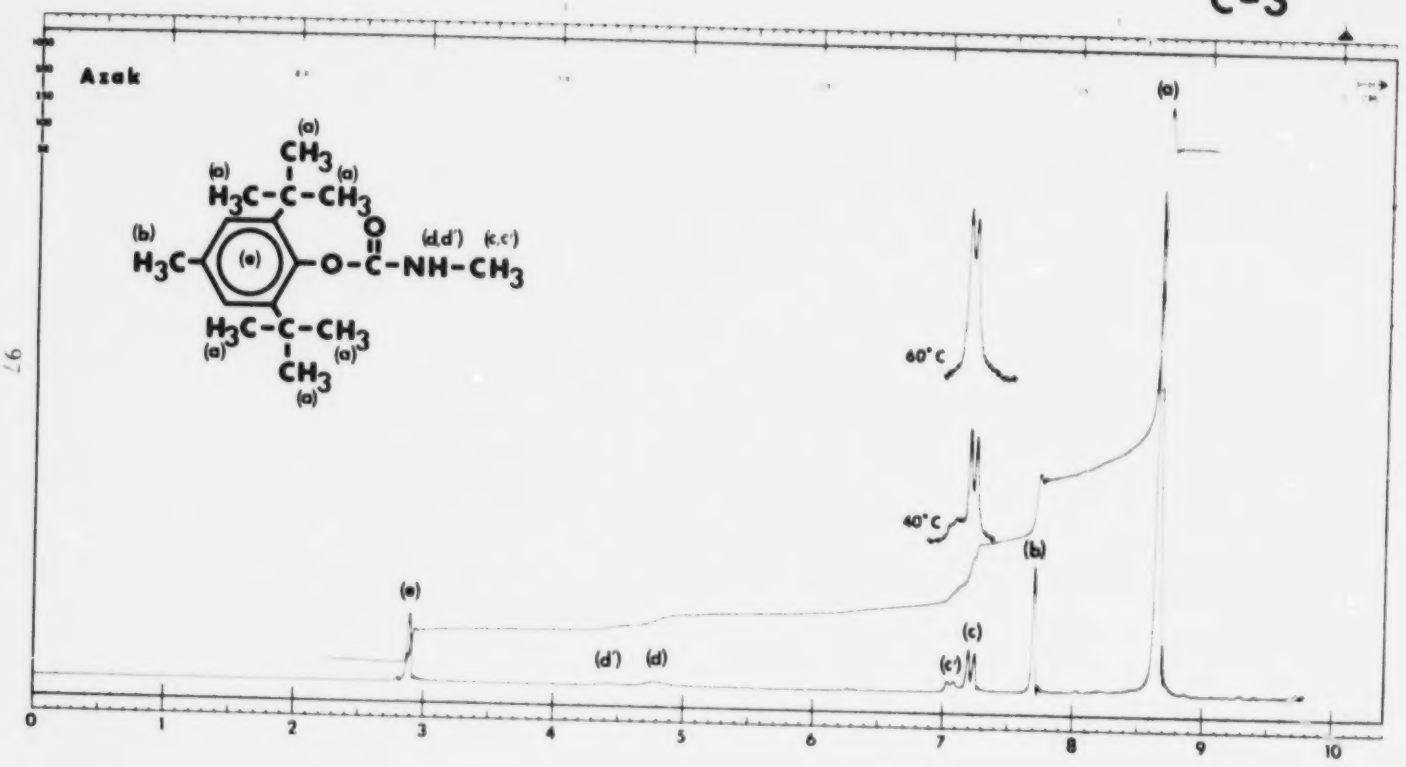
	T	J
a	7.91	
b	7.76	
c	7.26	5
d	4.7	
e	3.25	

C-2

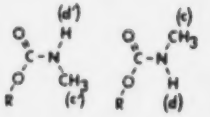


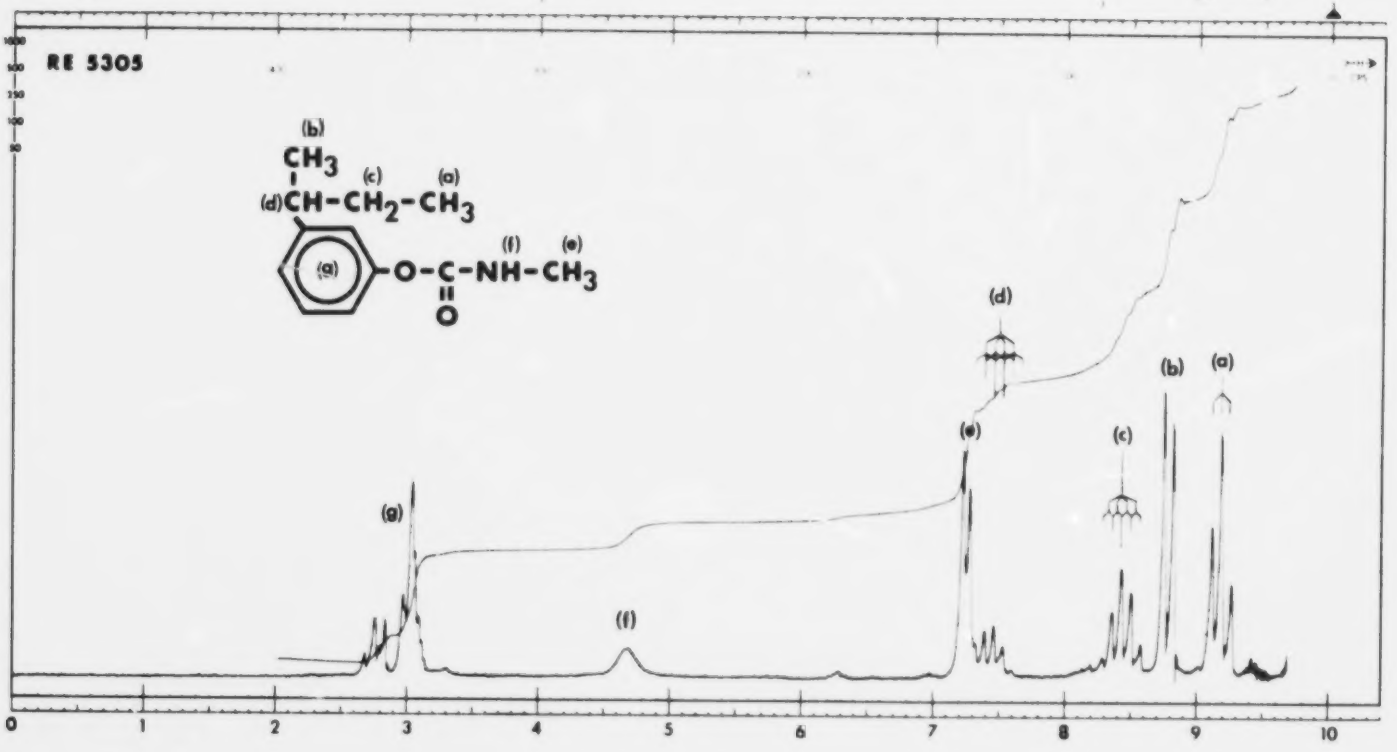
	T	J
a	8.77	7
b	7.26	5
c	7.12	7
d	4.6	
•	2.6-3.2	

C-3



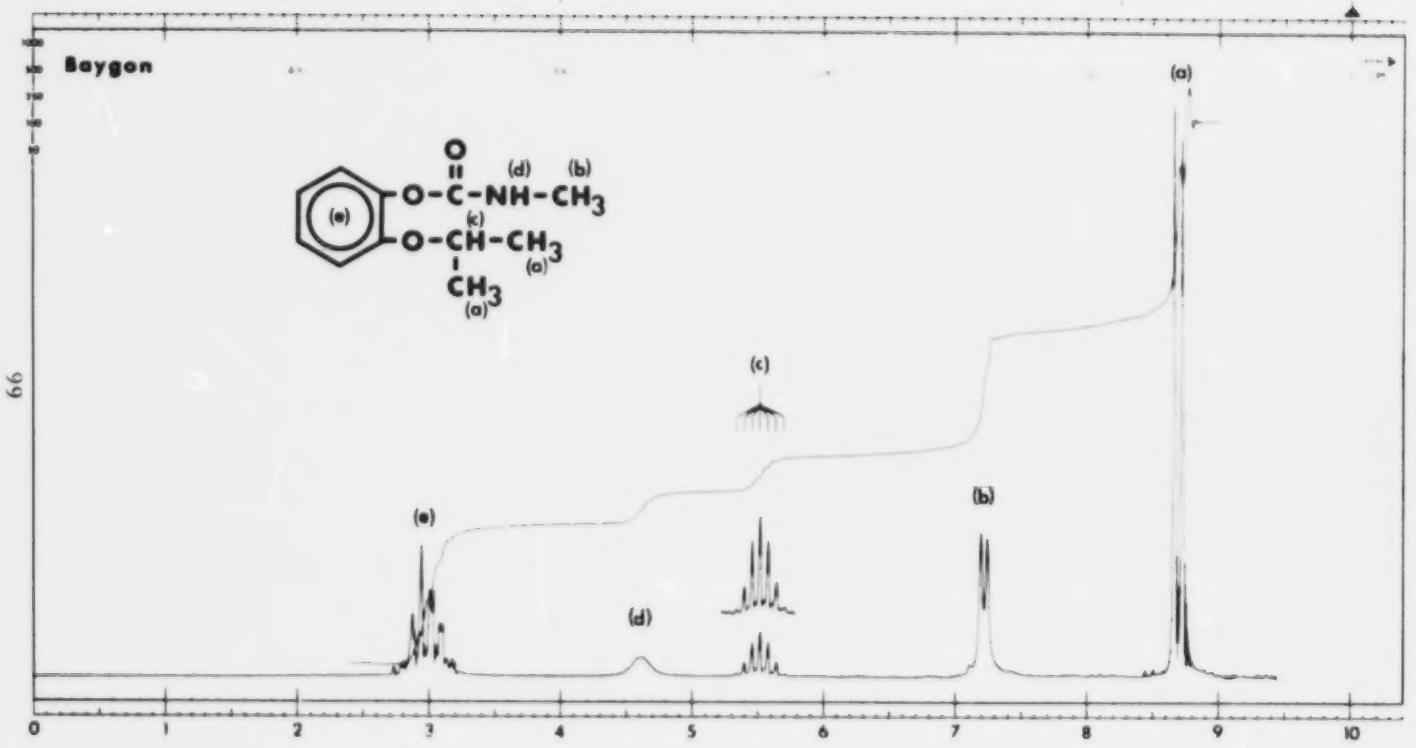
	T	J
a	8.64	
b	7.65	
c	7.22	5
c'	7.06	5
d'	4.8	
d	4.4	
e	2.88	





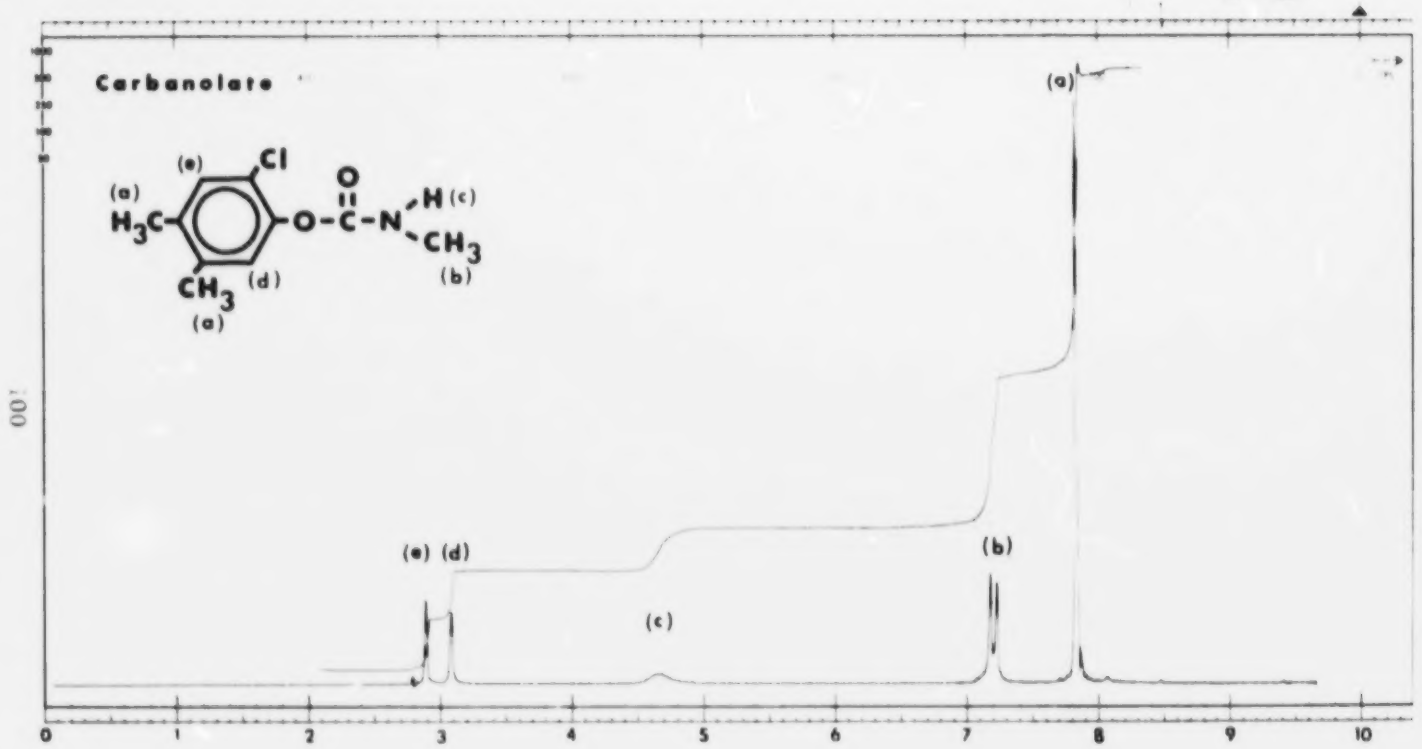
	T	J
a	9.19	7
b	8.78	7
c	8.43	7
d	7.50	7
e	7.25	5
f	4.5	
g	2.7-3.1	

C-5

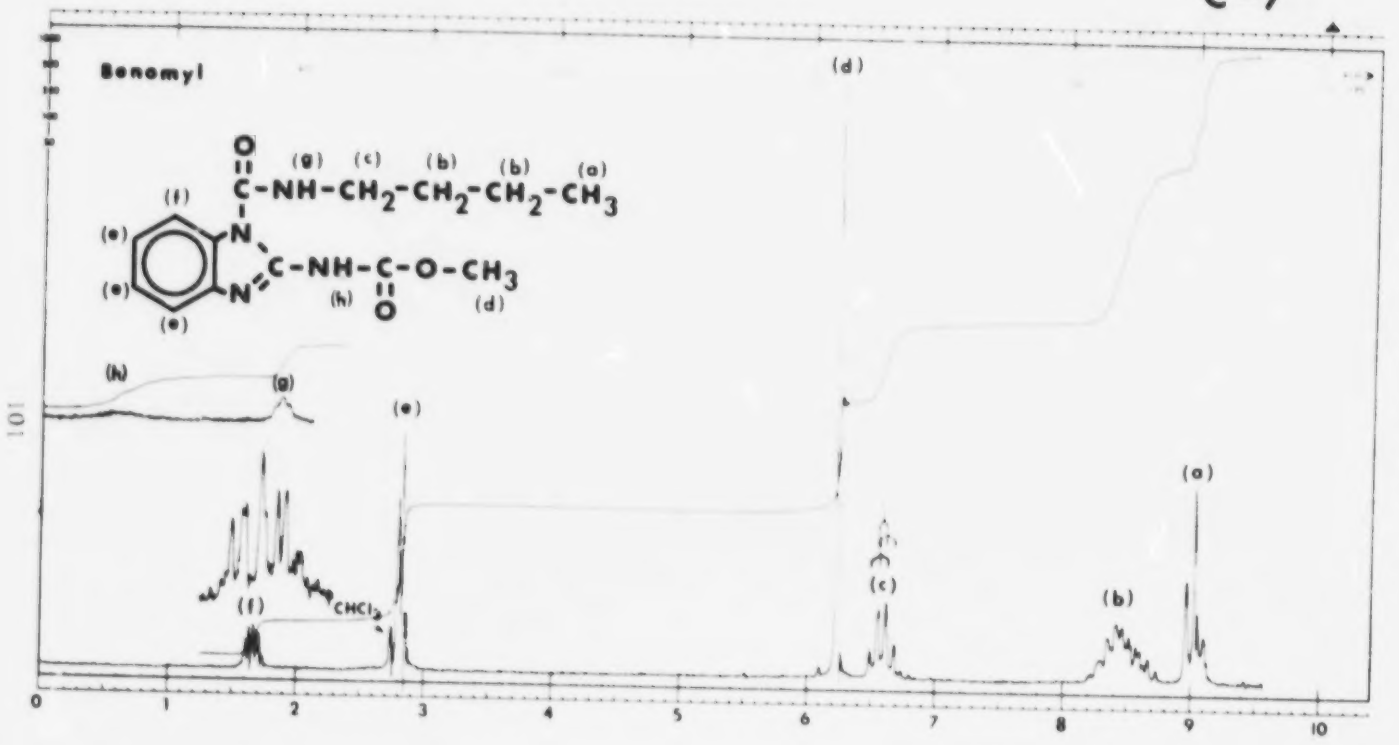


	T	J
a	8.70	6
b	7.22	5
c	5.52	6
d	4.6	
e	2.7-3.2	

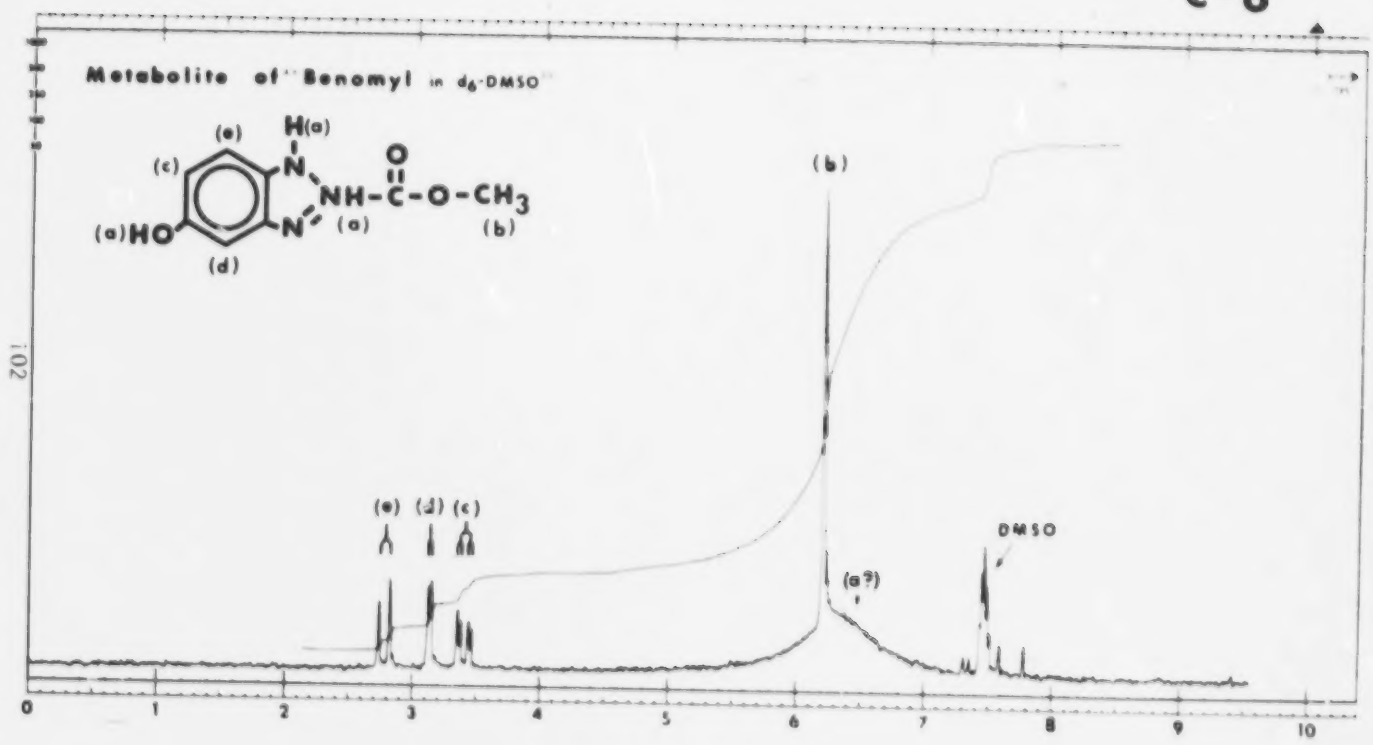
C-6



	T	J
a	7.83	
b	7.20	5
c	4.70	
d	3.07	
e	2.87	

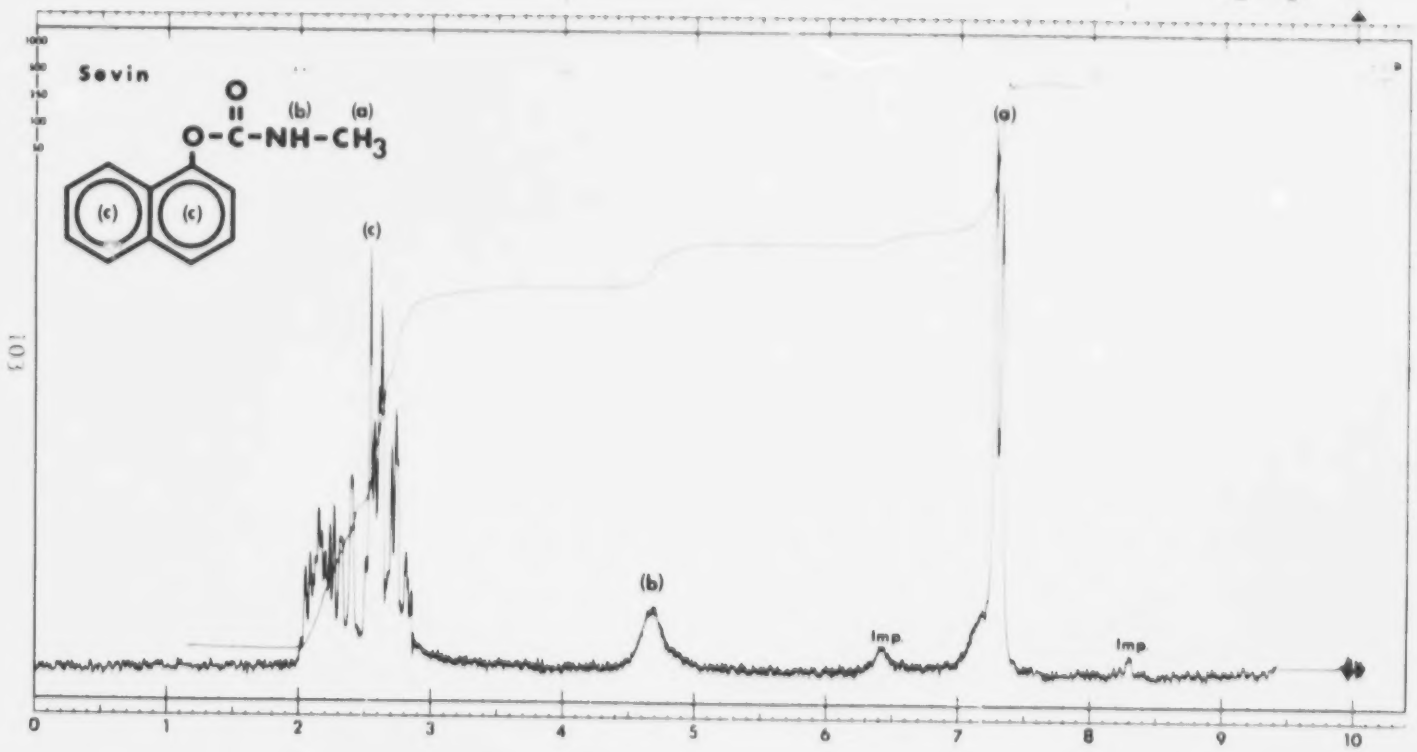


	T	J
a	9.02	7
b	8.2-8.7	
c	6.57	$\gamma(H_b-H_c)$
d	6.20	$\delta(H_c-H_g)$
e	2.80	
f	1.66	
g	- 0.14	
h	- 1.4	

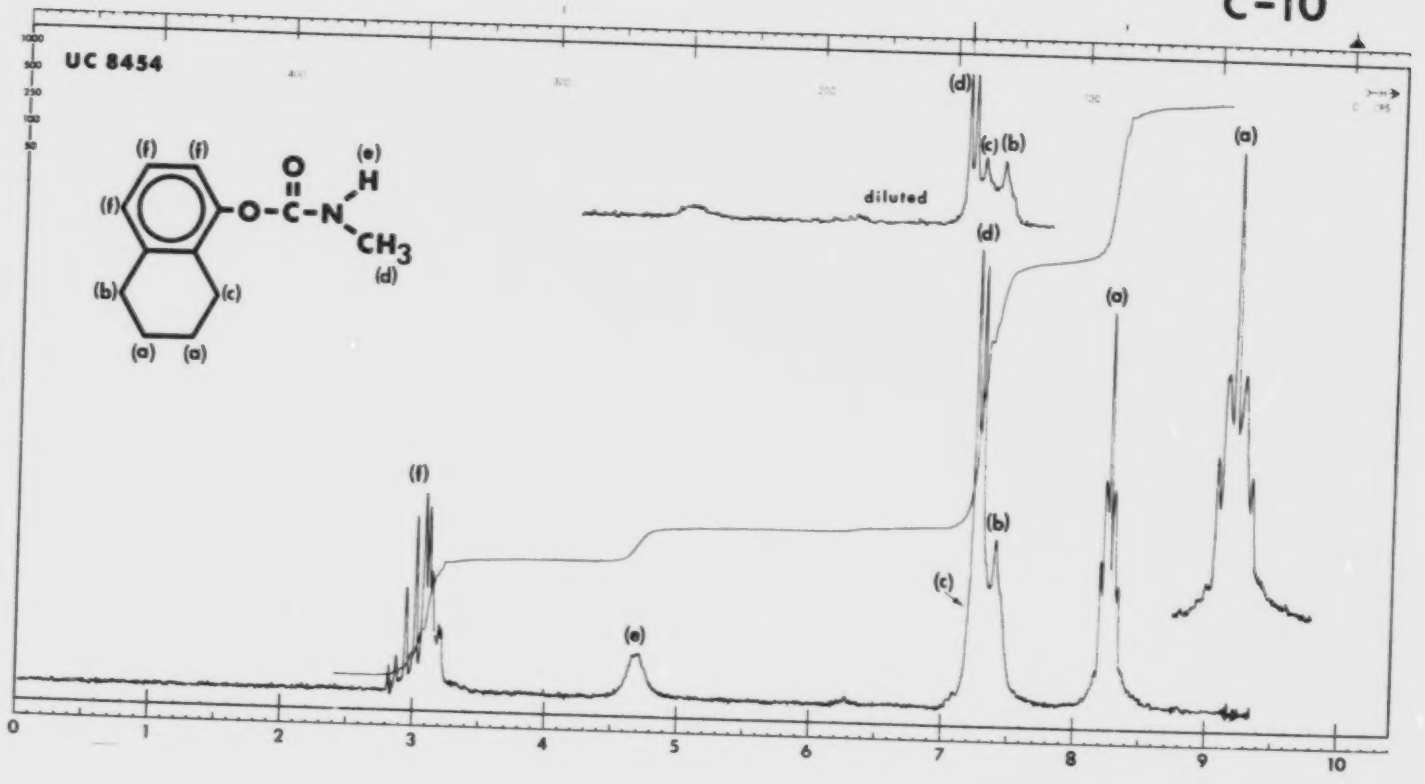


	T	J
a	6.30	
b	6.19	
c	3.40	8.5(H_c-H_e) 2.5(H_c-H_d)
d	3.12	2.5(H_c-H_d)
e	2.76	4.5(H_c-H_e)

C-9

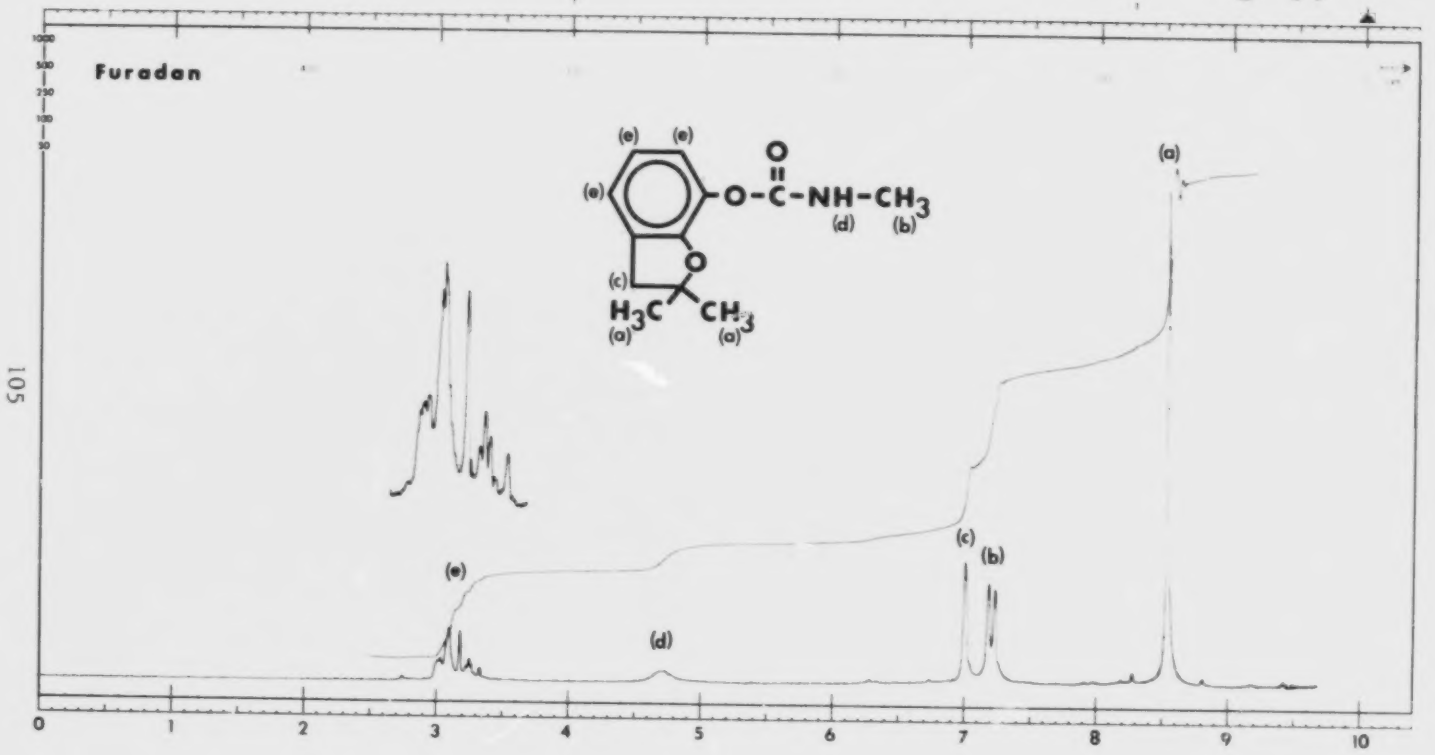


	τ	J
a	7.29	5
b	4.7	
c	2.0-2.8	



	T	J
a	8.24	
b	7.38	
c	7.2	
d	7.24	5
e	4.7	
f	2.9-3.2	

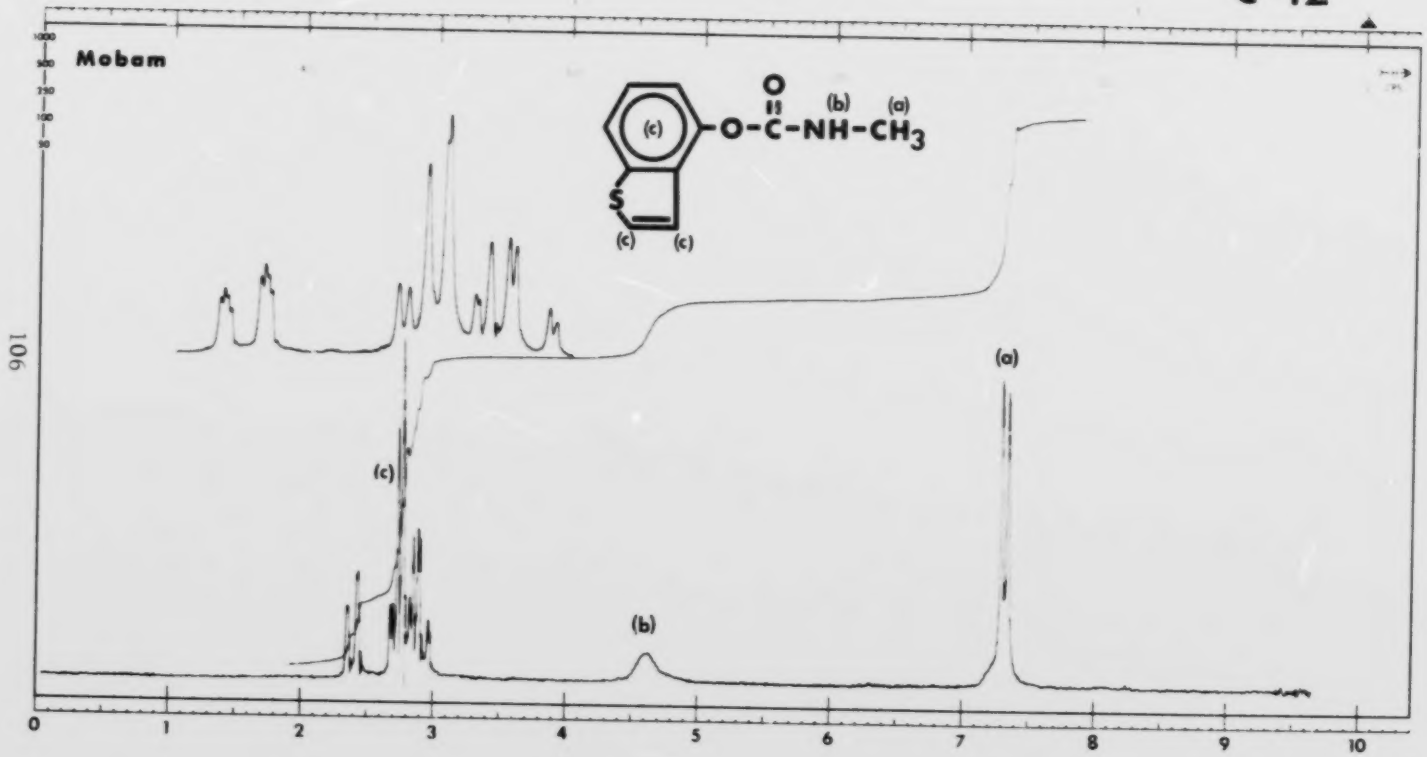
C-11



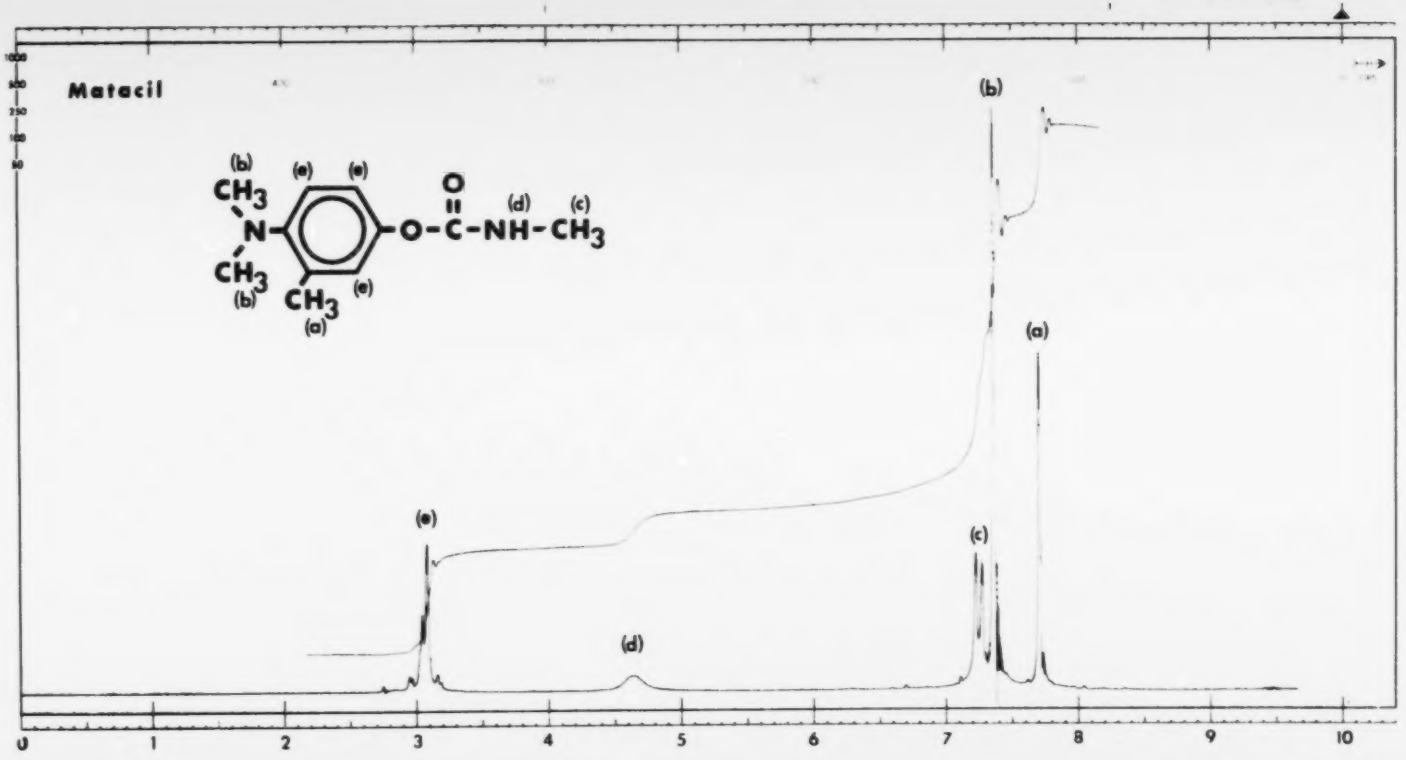
105

	T	J
a	8.52	
b	7.20	5
c	7.00	
d	4.7	
e	3.0-3.3	

C-12

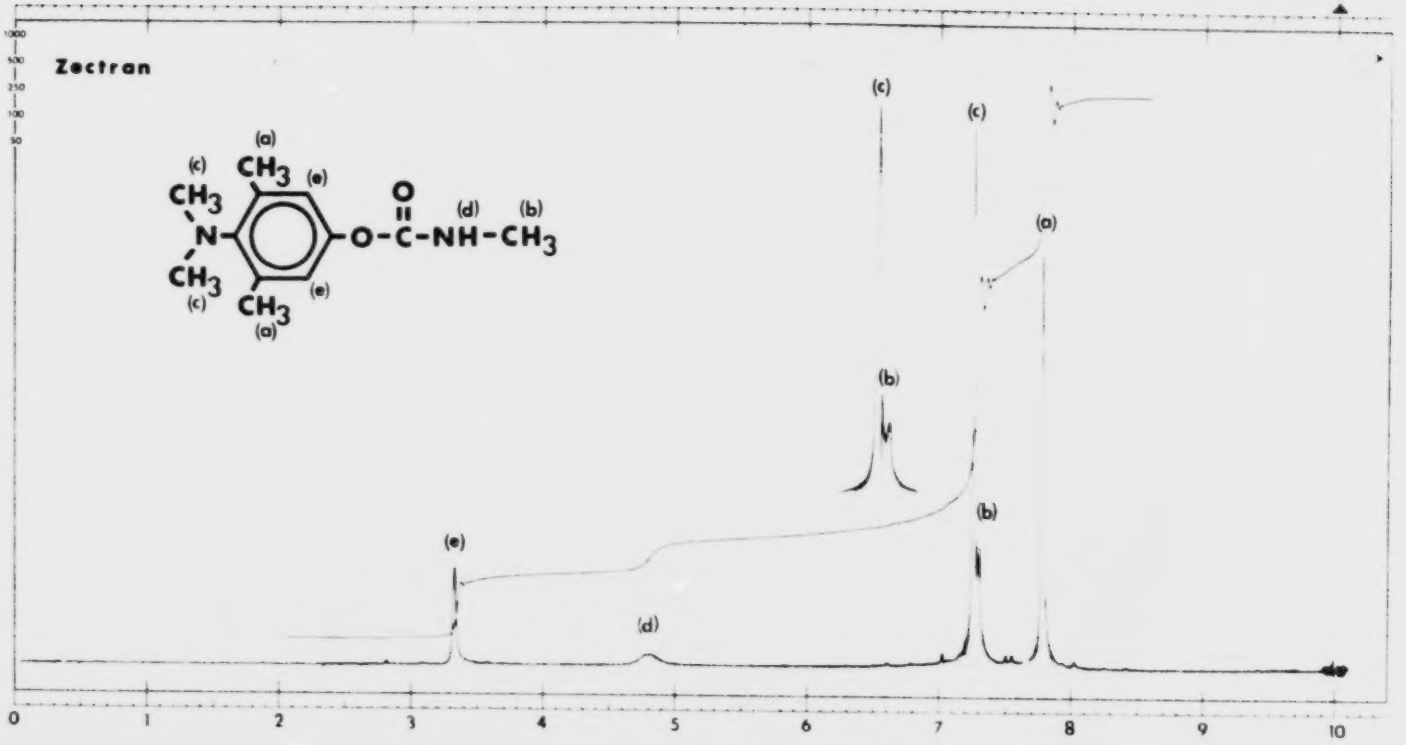


	T	J
a	7.32	5
b	4.59	
c	2.3-3.0	



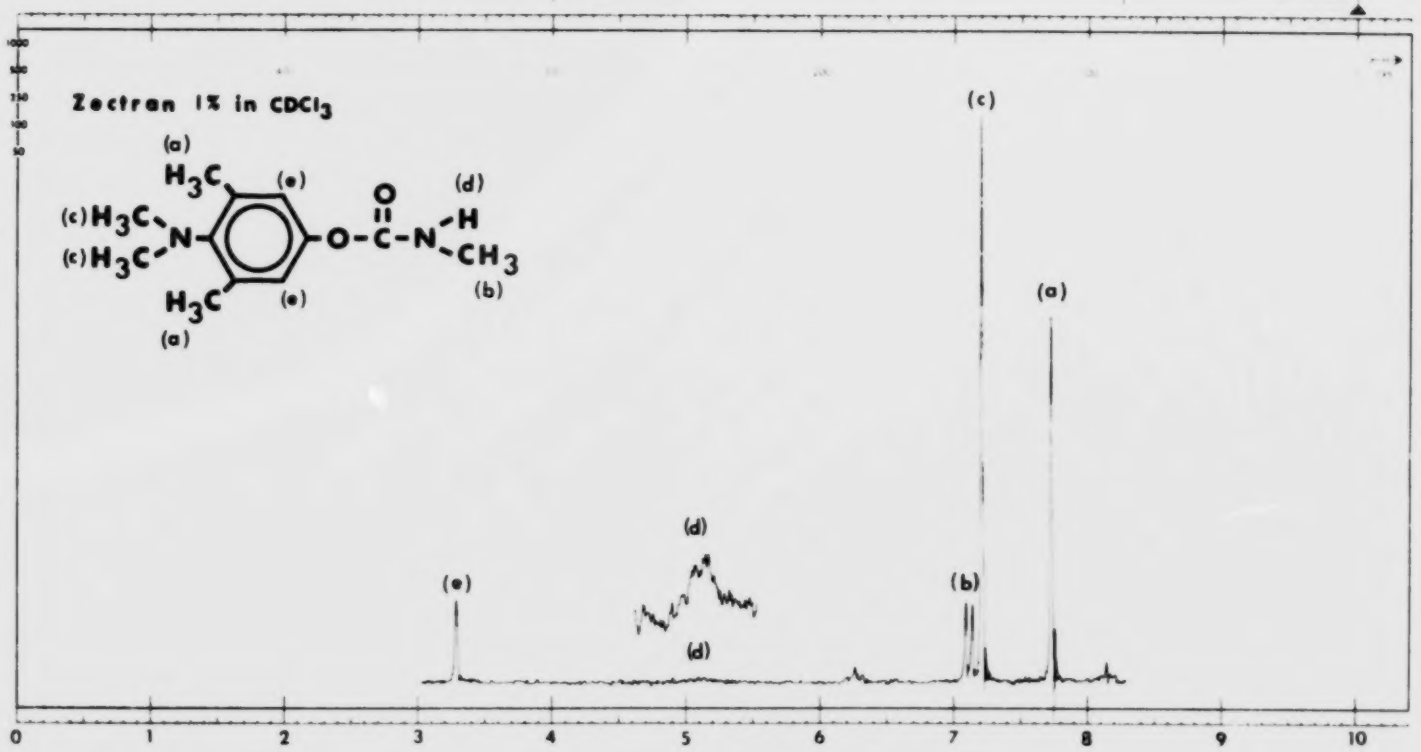
	T	J
a	7.71	
b	7.37	
c	7.26	5
d	4.6	
e	3.1	

C-14a



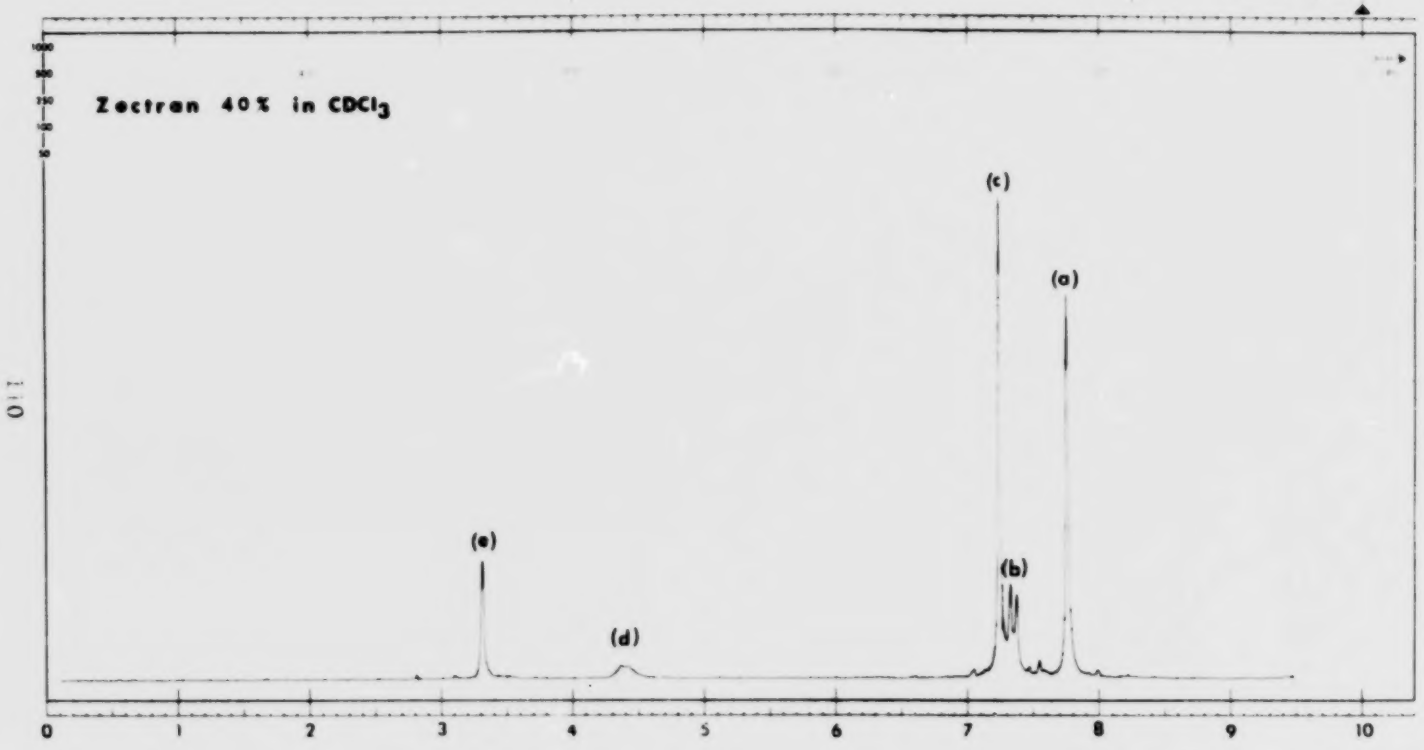
	T	J
a	7.88	
b	7.28	5
c	7.26	
d	4.80	
e	3.33	

C-14b

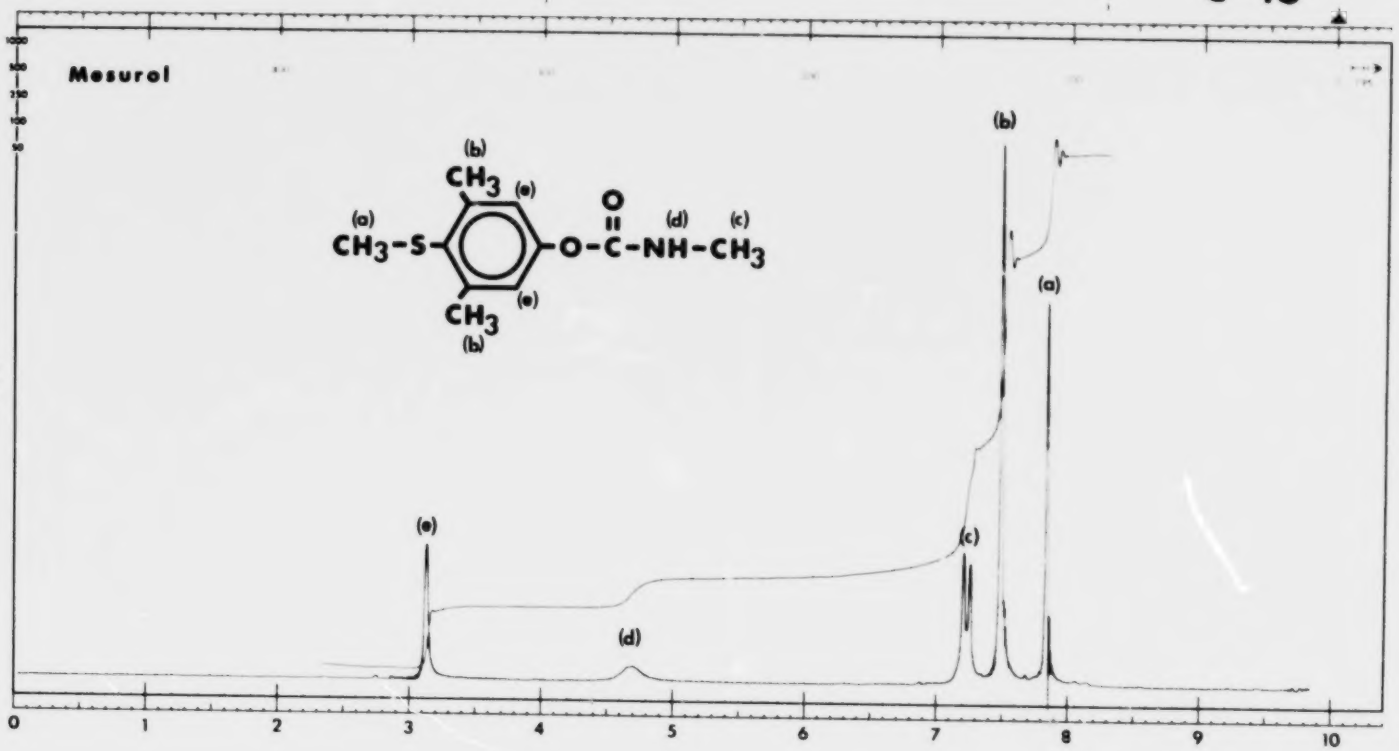


	T	J
a	7.75	
b	7.1-7.15	5
c	7.22	
d	5.14	
e	3.28	

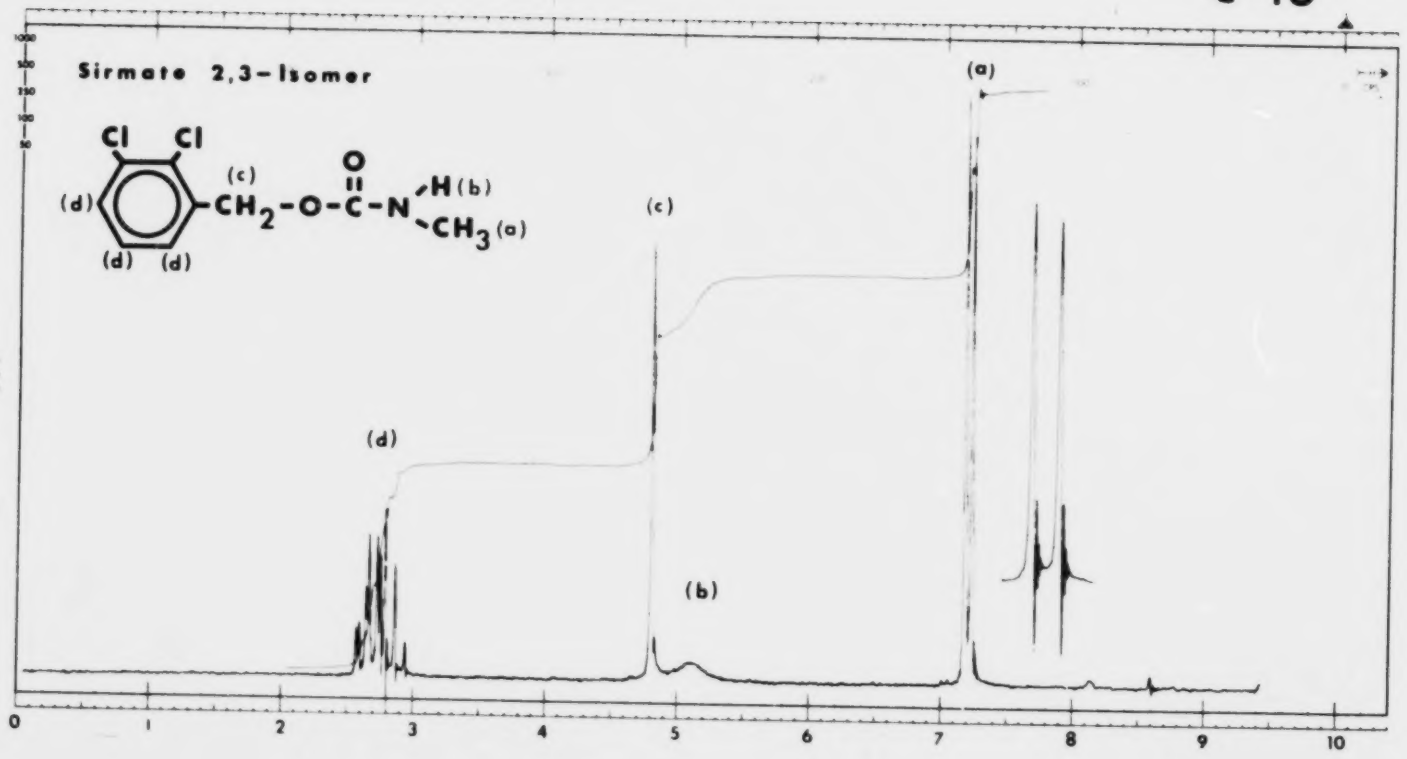
C-14c



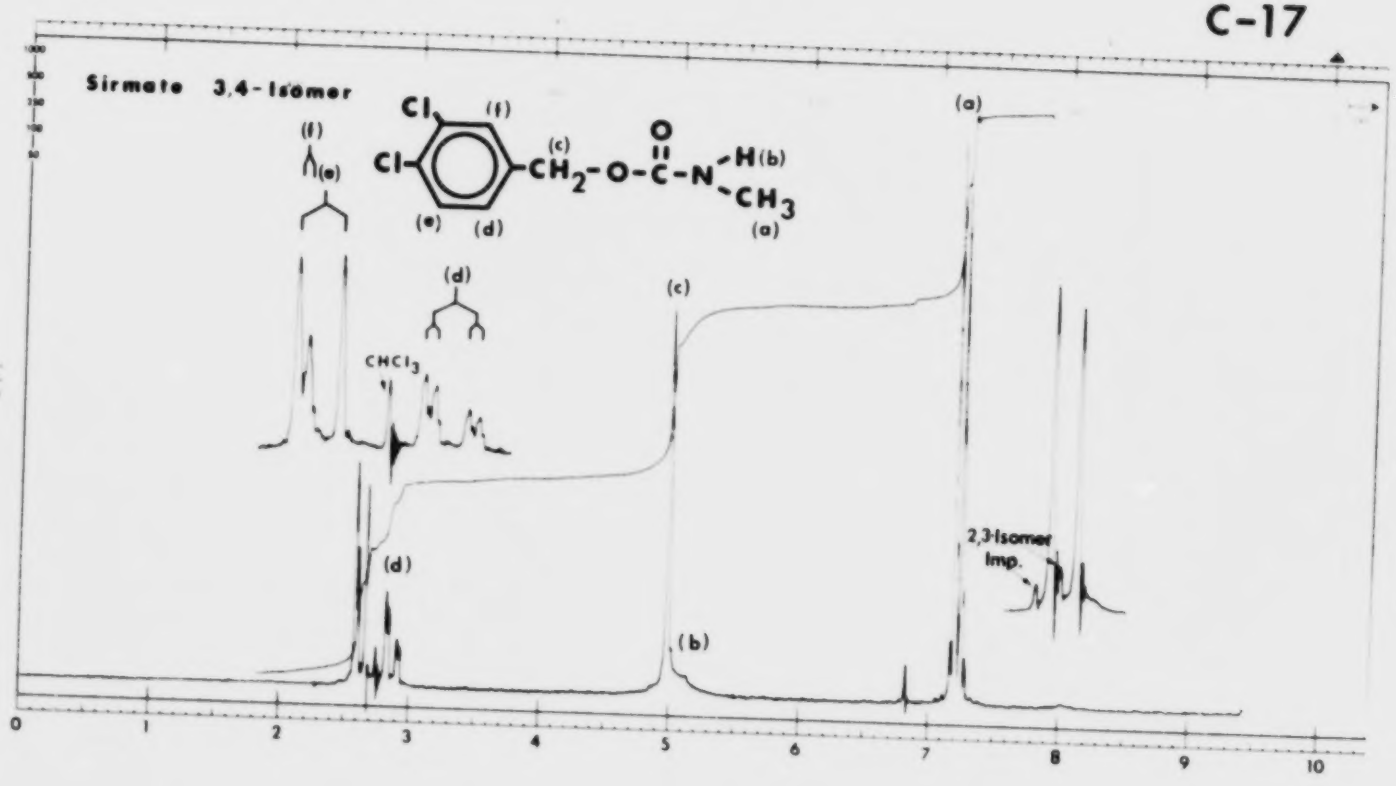
	T	J
a	7.78	
b	7.33–7.38	5
c	7.25	
d	4.39	
e	3.31	



	T	J
a	7.93	
b	7.48	
c	7.24	5
d	4.7	
e	3.13	



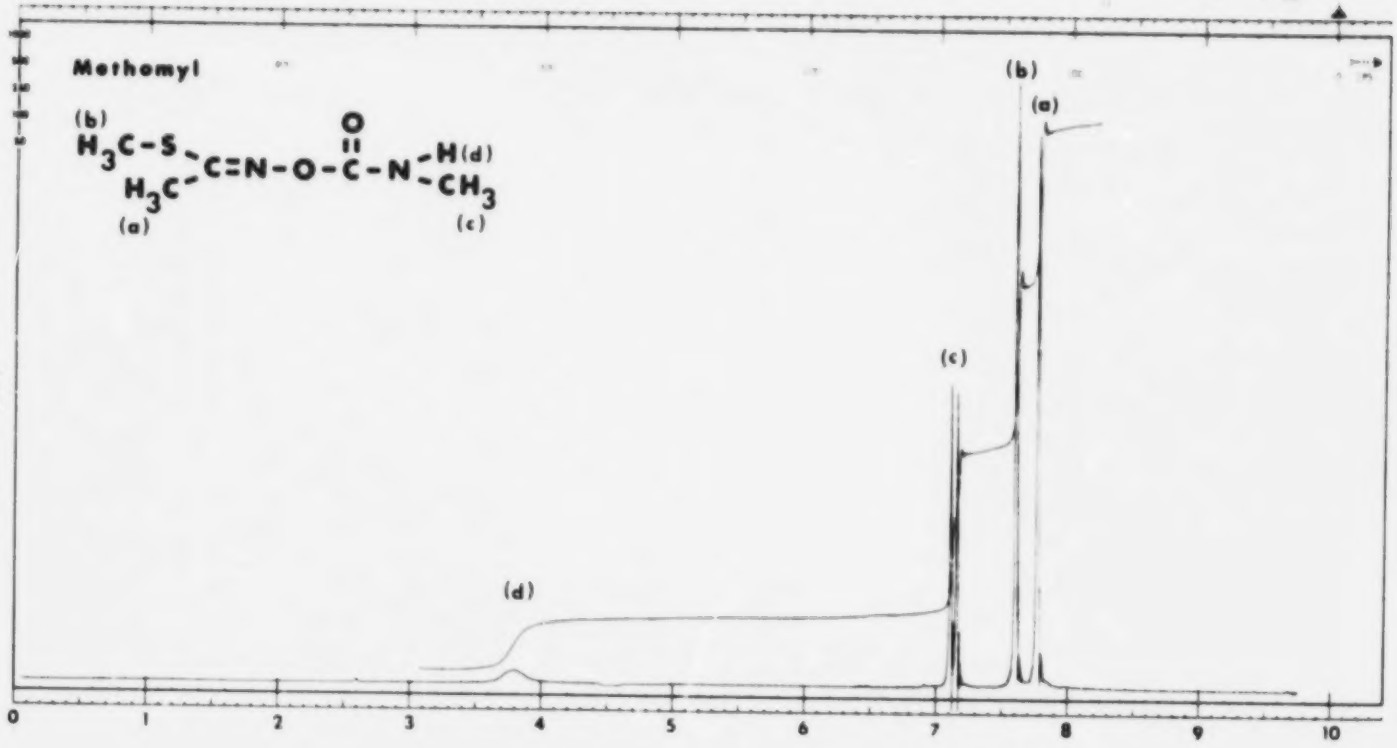
	T	J
a	7.18	5
b	5.10	
c	4.78	
d	2.55 - 2.92	



	T	J
a	7.20	5
b	5.0	
c	4.97	
d	2.86	8.5(H_d-H_e)
		2.0(H_d-H_f)
e	2.61	8.5(H_d-H_e)
f	2.58	2.0(H_d-H_f)

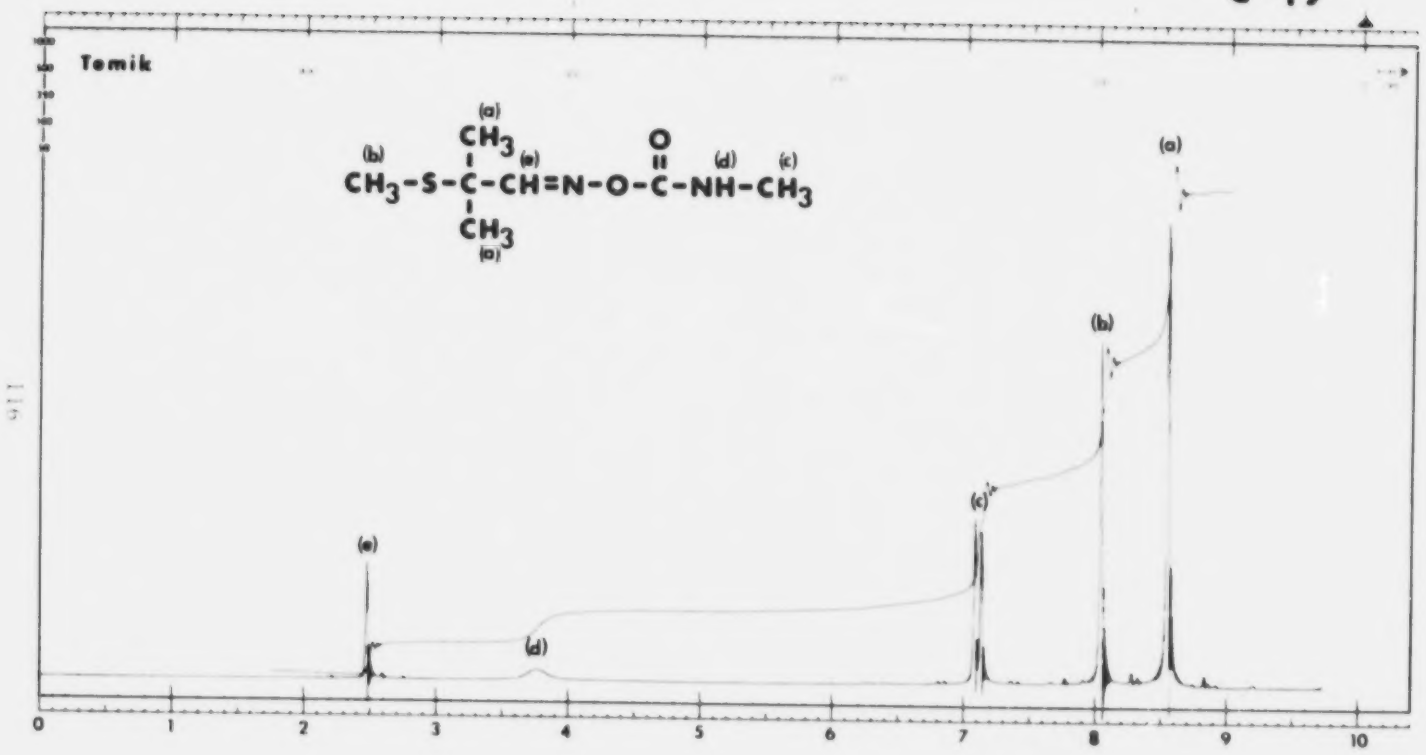
C-17b

Commercial Silmate
Mixture
80% 3,4 Isomer
20% 2,3 Isomer
0
1
2
3
4
5
6
7
8
9
10



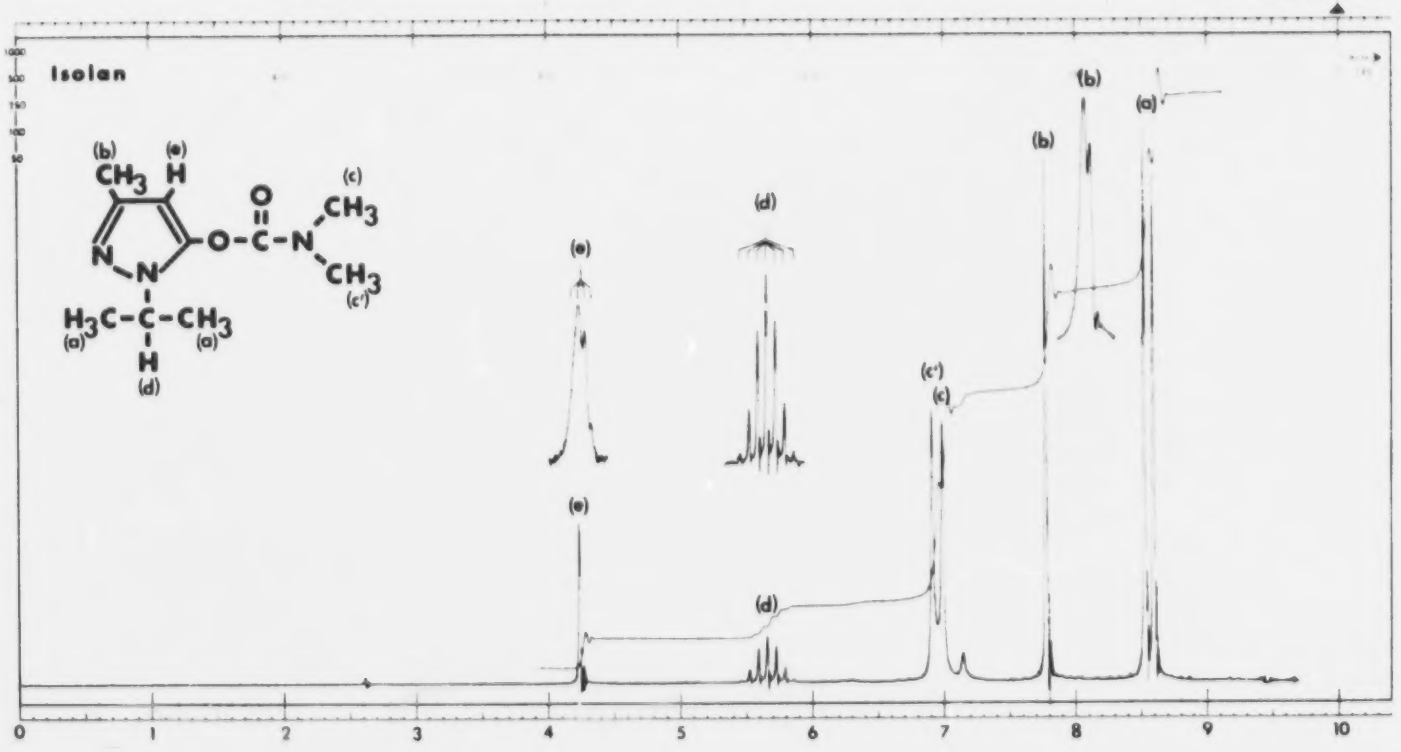
	T	J
a	7.77	
b	7.61	
c	7.13	5
d	3.80	

C-19



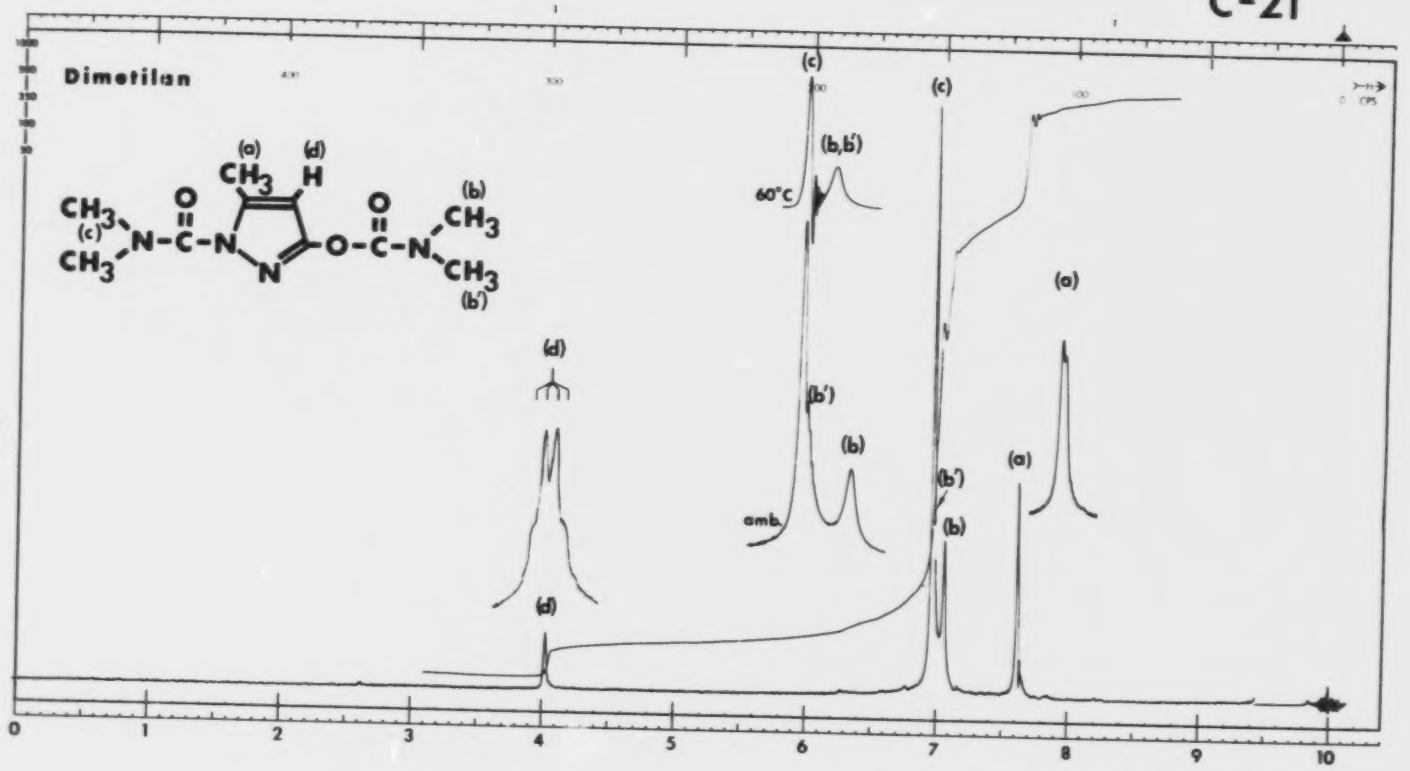
	T	J
a	8.54	
b	8.03	
c	7.10	5
d	3.75	
e	2.46	

C-20



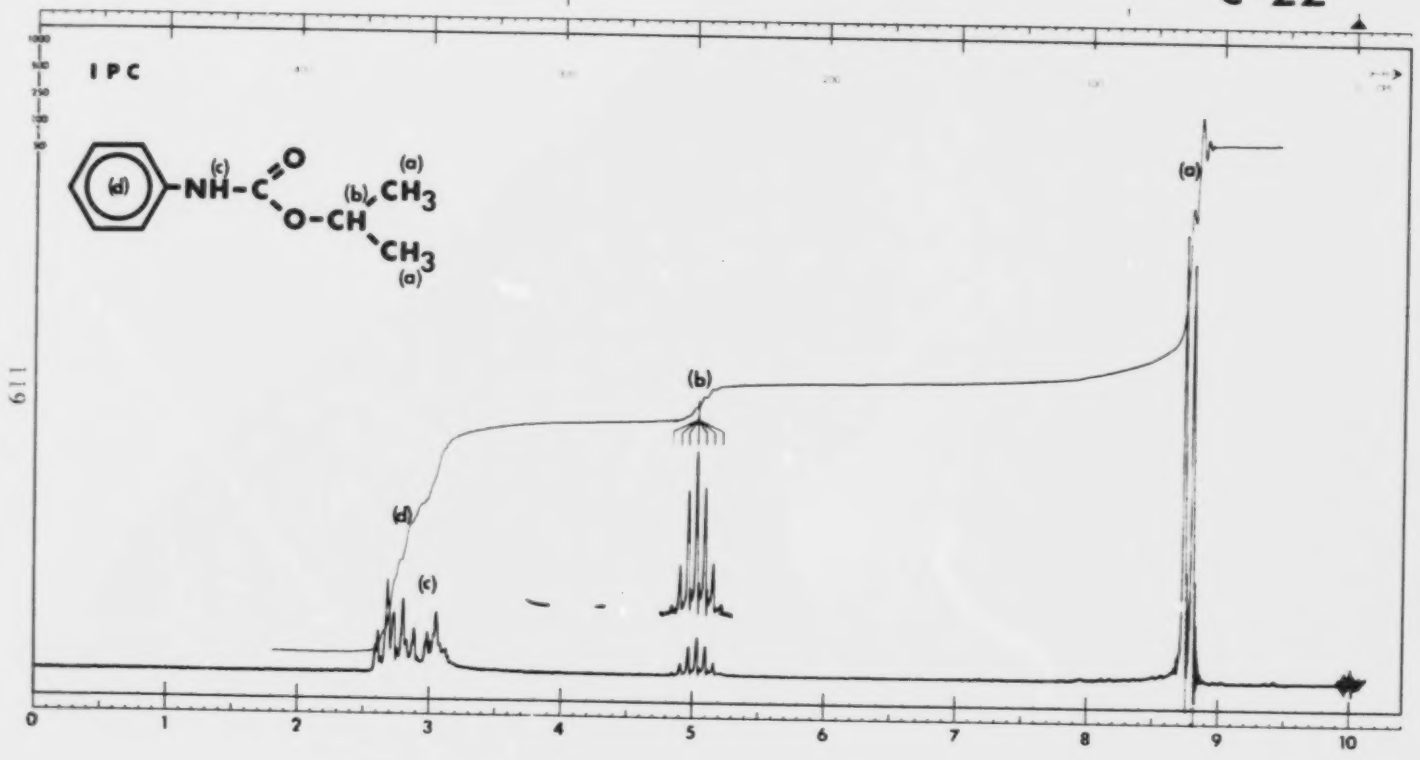
	T	J
a	8.57	7
b	7.78	0.5
c	6.99	
c'	6.91	
d	5.66	7
e	4.23	0.5

C-21



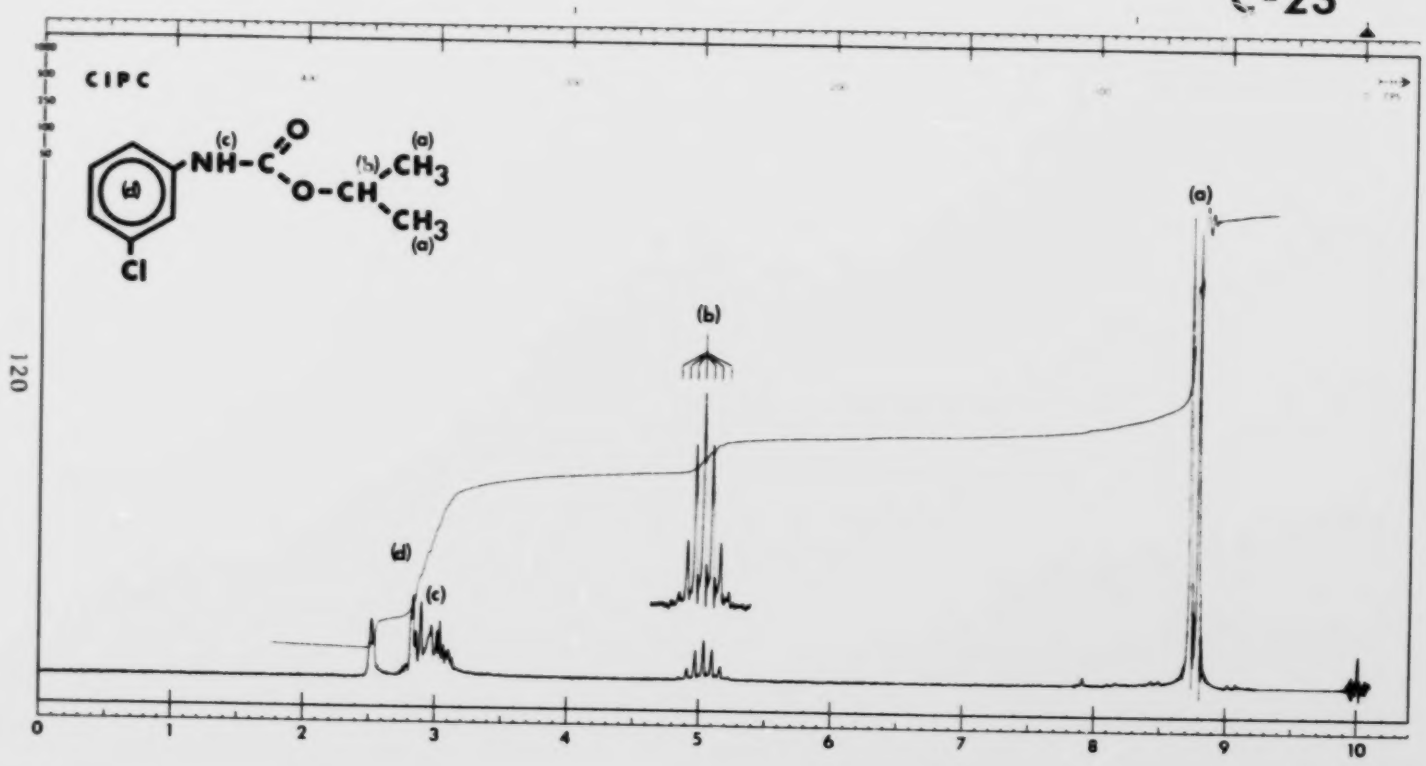
	T	J
a	7.60	0.8
b	7.03	
b'	6.95	
c	6.94	
d	3.99	0.8

C-22



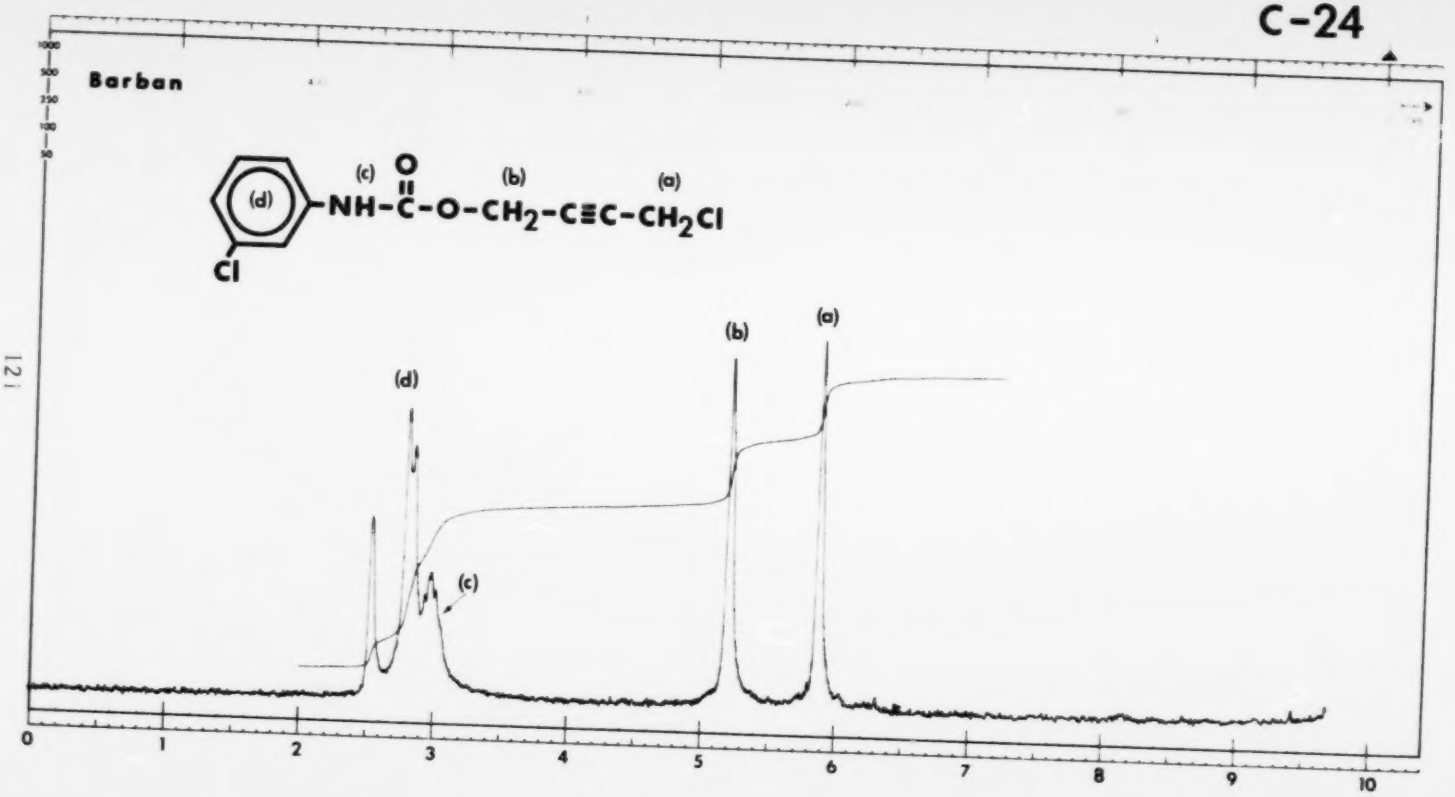
	T	J
a	8.76	6
b	5.00	6
c	3.0	
d	2.6-3.1	

C-23



	T	J
a	8.75	6
b	5.03	6
c	3.0	
d	2.5-3.1	

C-24

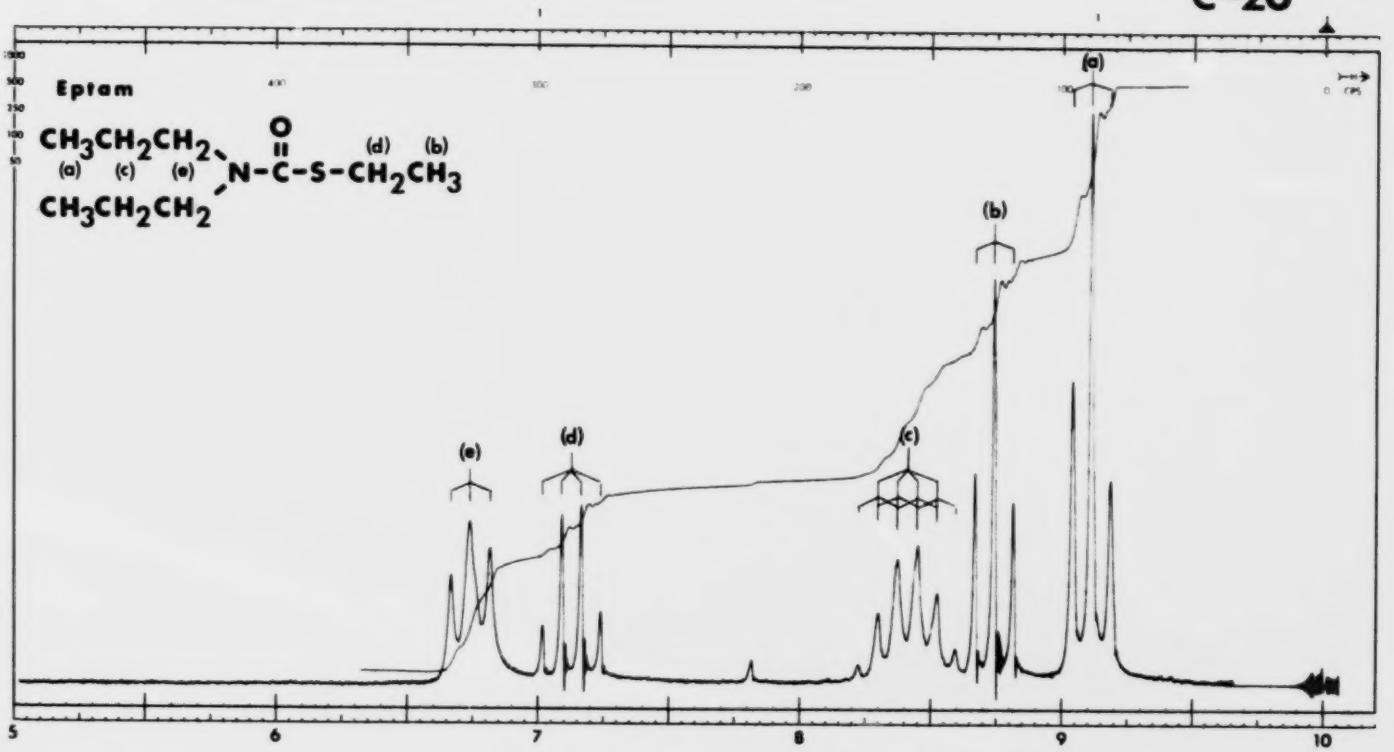


	T
a	5.86
b	5.20
c	2.9
d	2.5-3.0

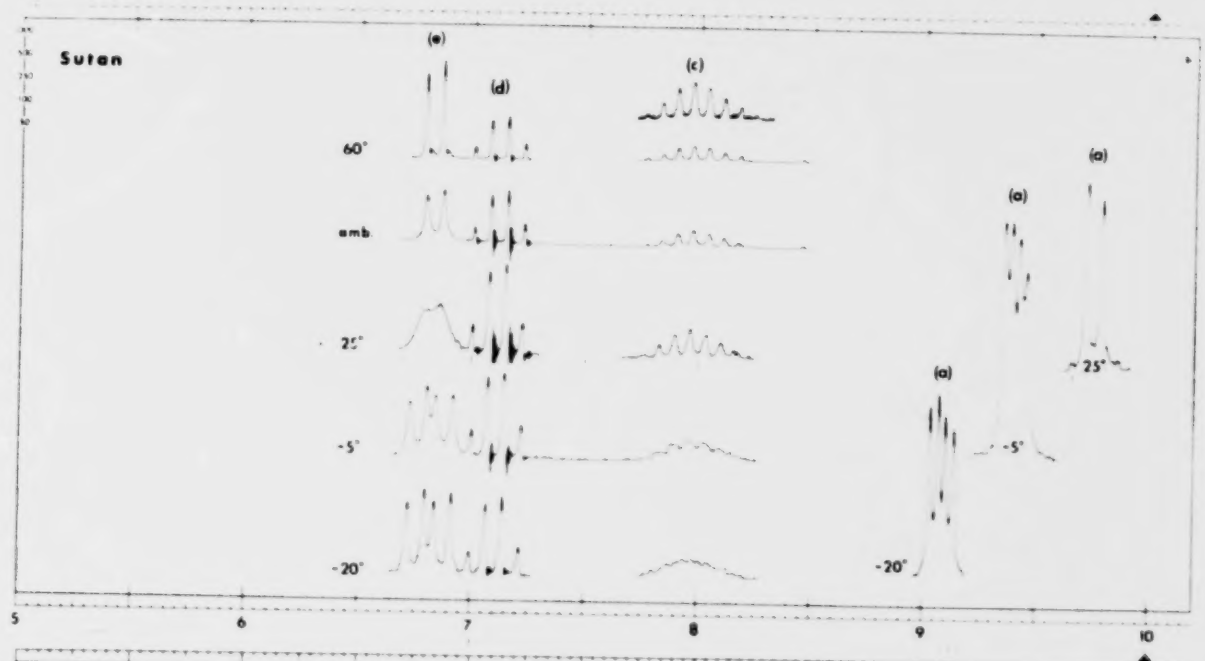
C-25

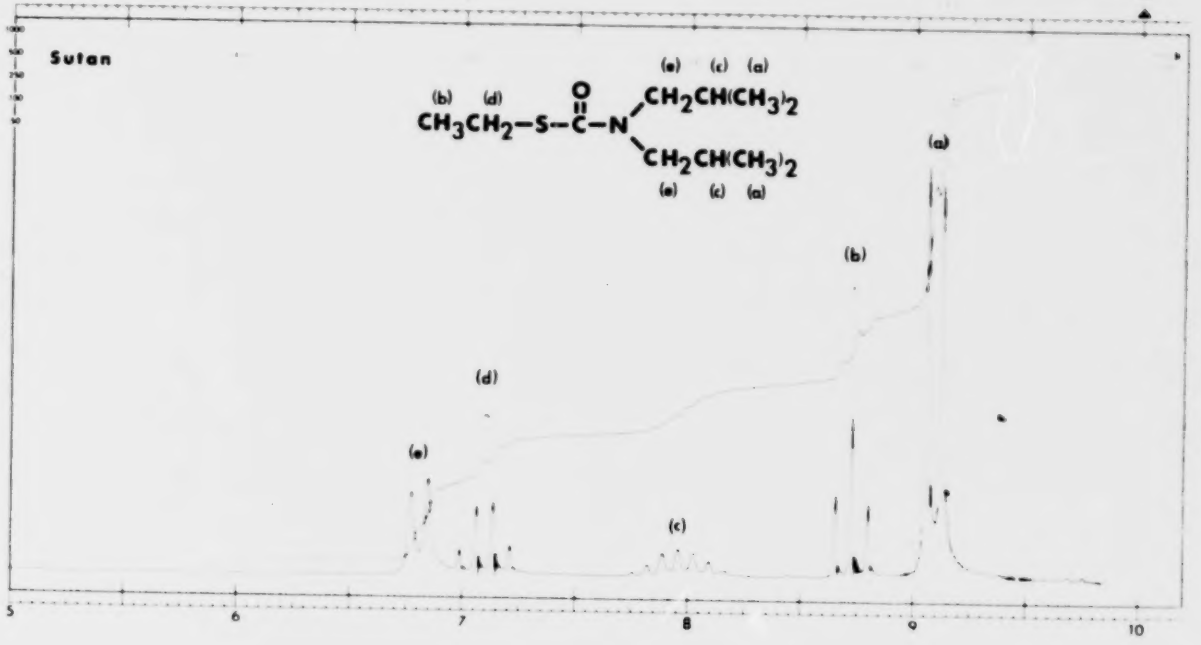
	T
a	6.25
b	3.05
c	2.4-2.9

C-26

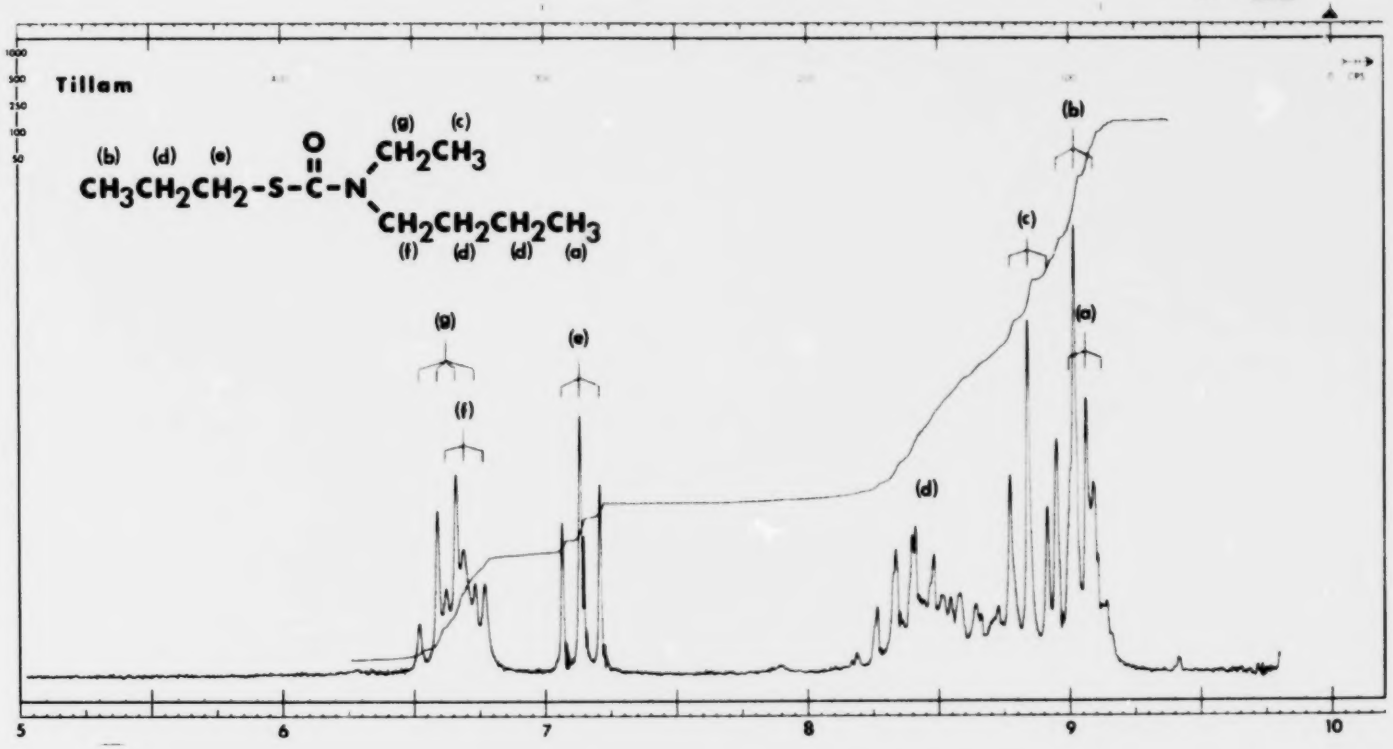


	T	J
a	9.10	7
b	8.73	7.5
c	8.40	7-7.5
d	7.11	7.5
e	6.72	7.5

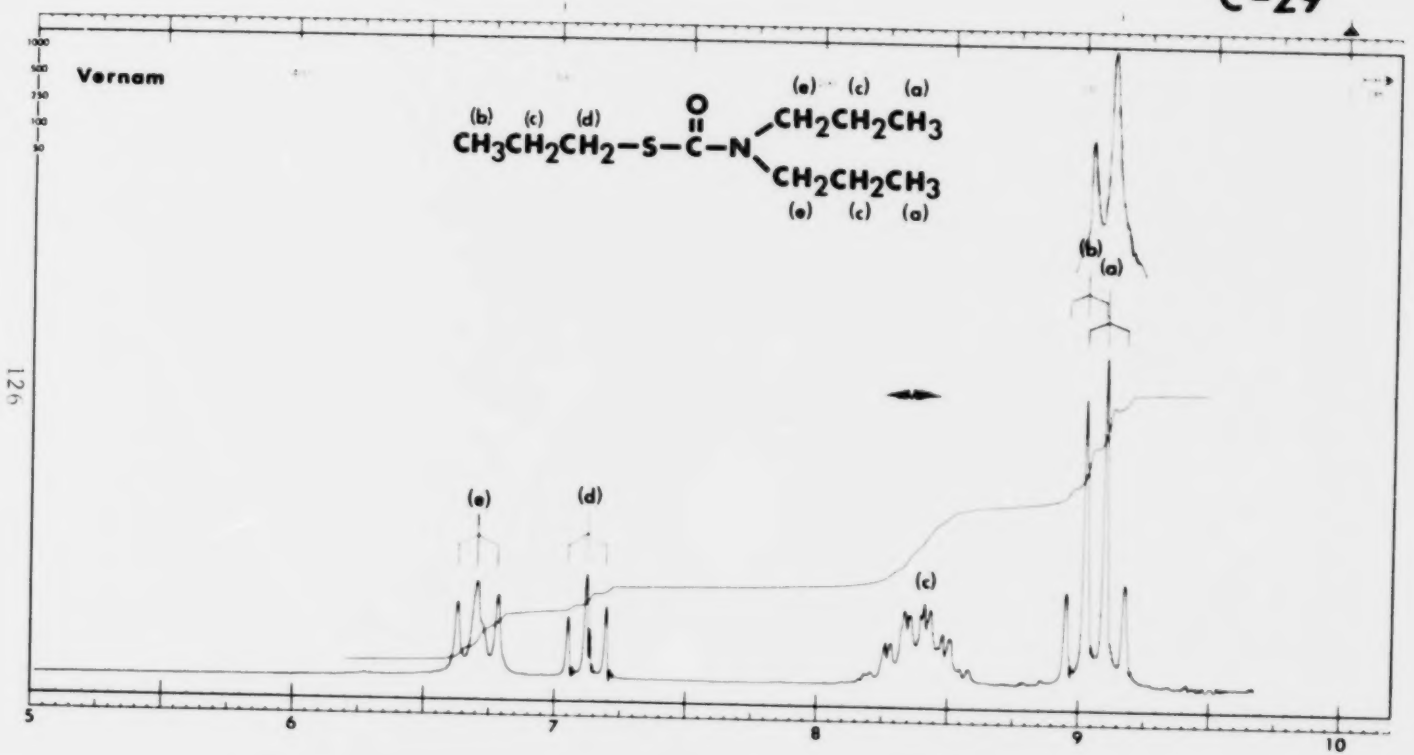




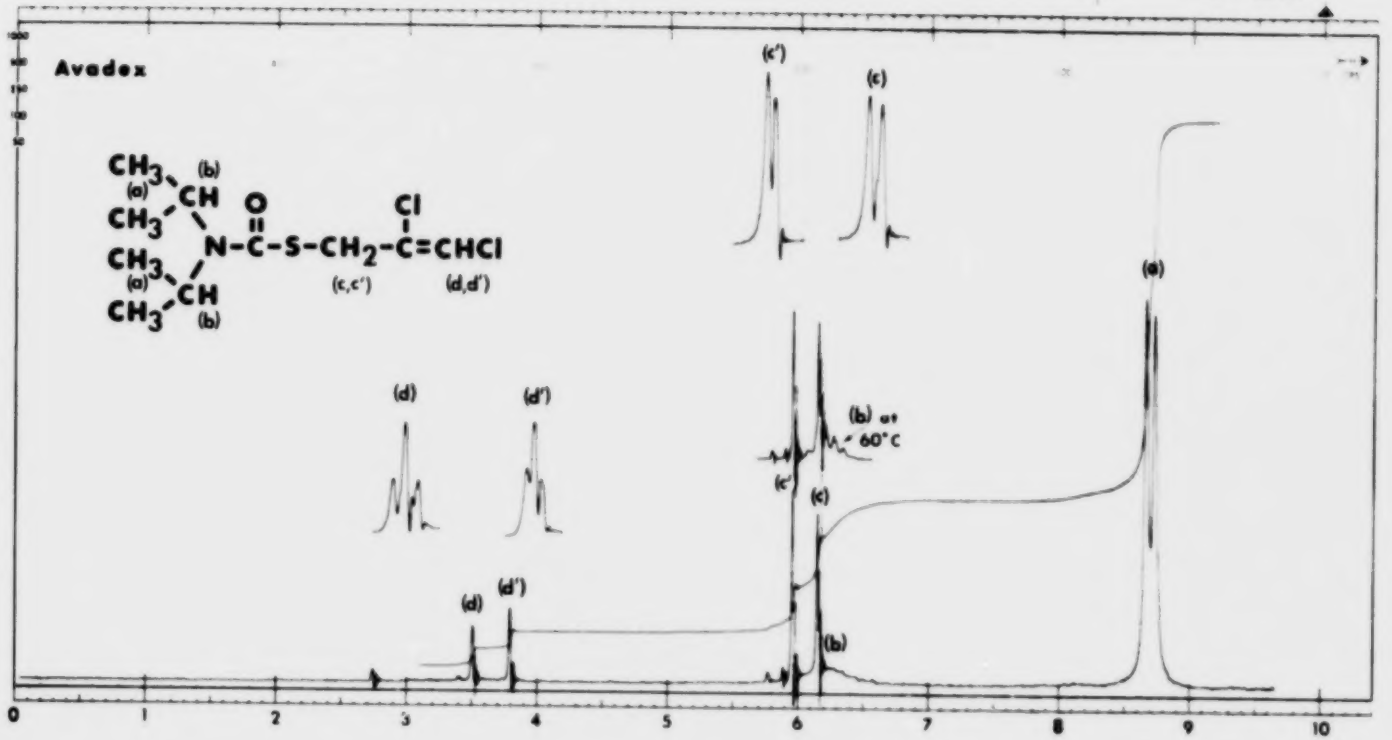
	T	J
a	9.09	6.5
b	8.75	7
c	7.96	
d	7.10	7
e	6.81	7.5



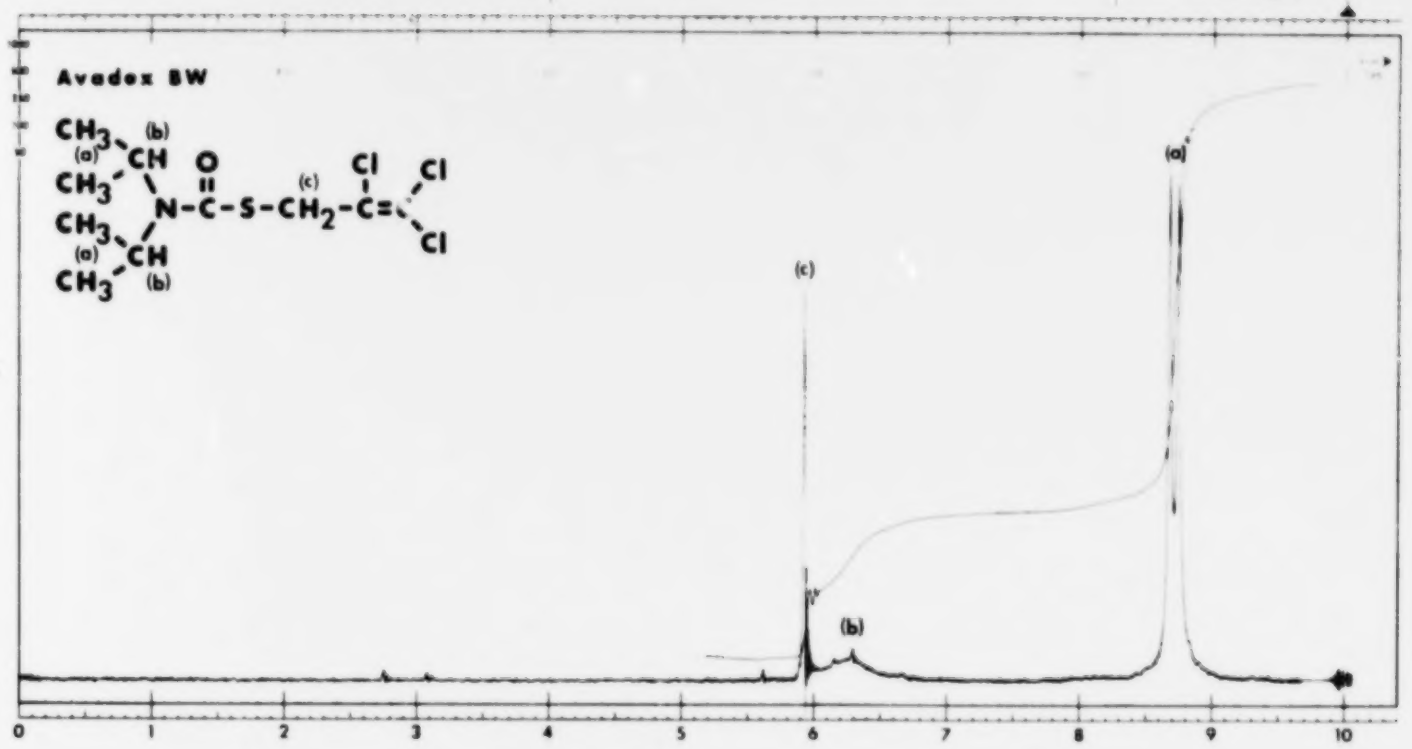
	T	J
a	9.08	6.5
b	9.03	7
c	8.86	7
d	8.2–8.7	
e	7.15	7
f	6.70	7
g	6.64	7



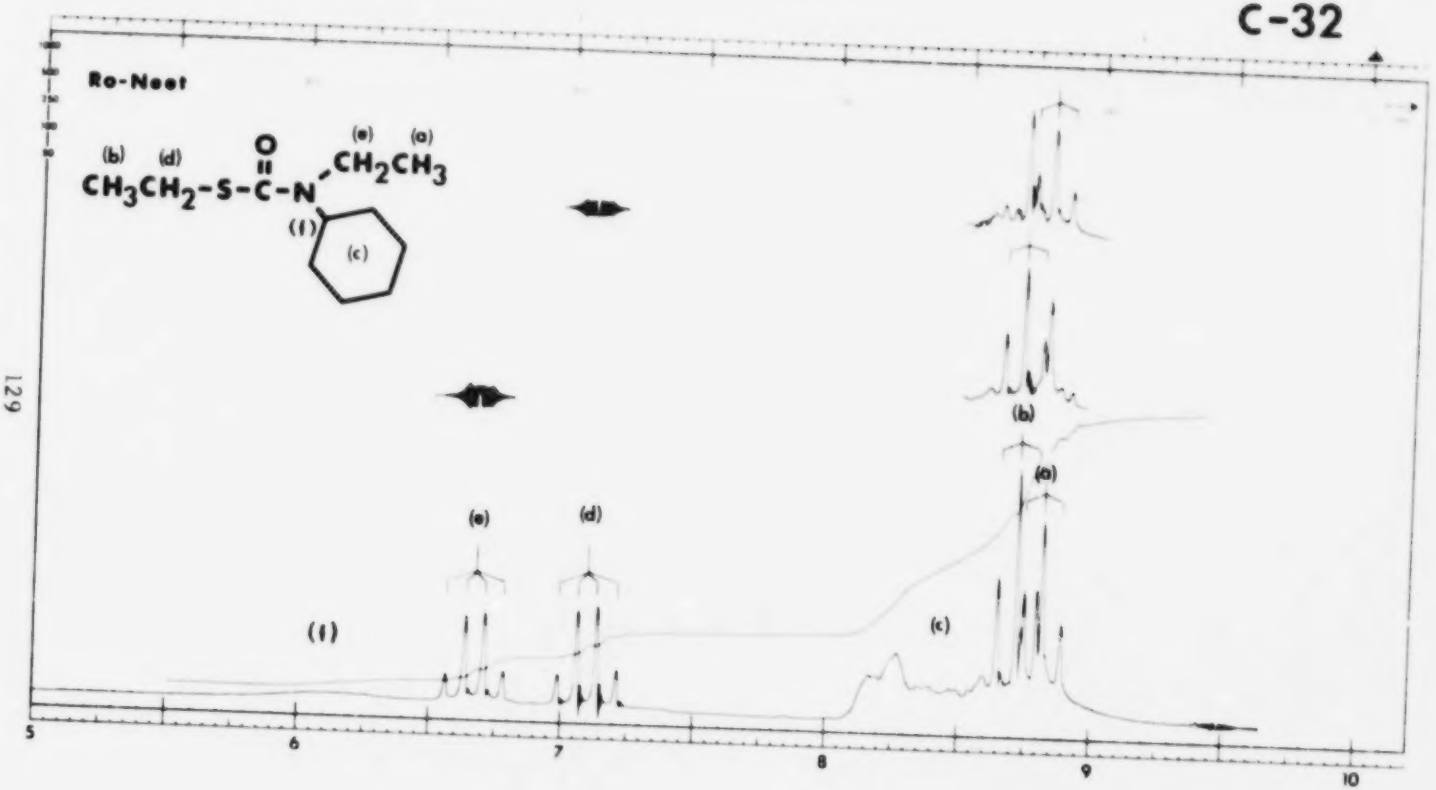
	T	J
a	9.10	7.5
b	9.02	7
c	8.2–8.6	
d	7.12	7
e	6.71	7.5



	T	J
a	8.70	7
b	6.2	
c	6.15	1.0
c'	5.96	0.6
d	3.78	0.6
d'	3.49	1.0

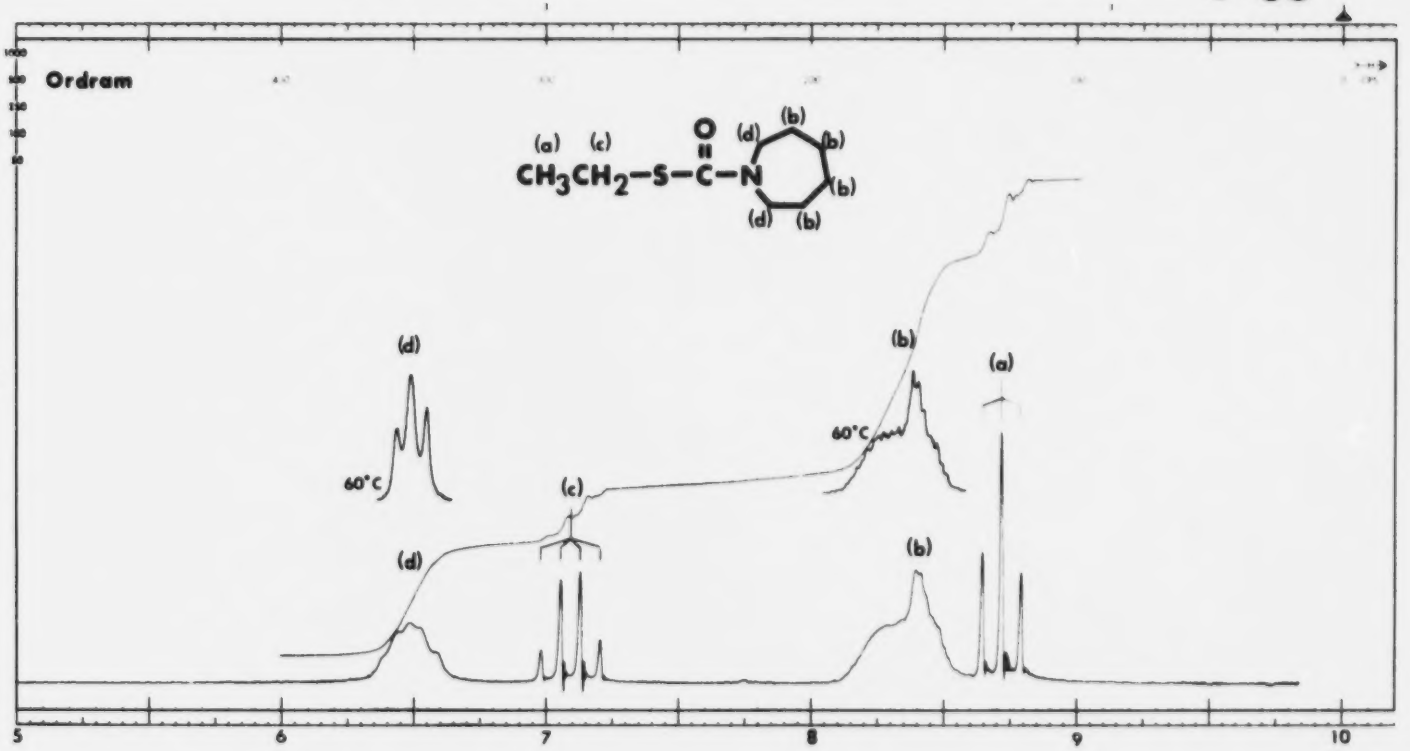


	T	J
a	8.71	7
b	6.3	
c	5.90	



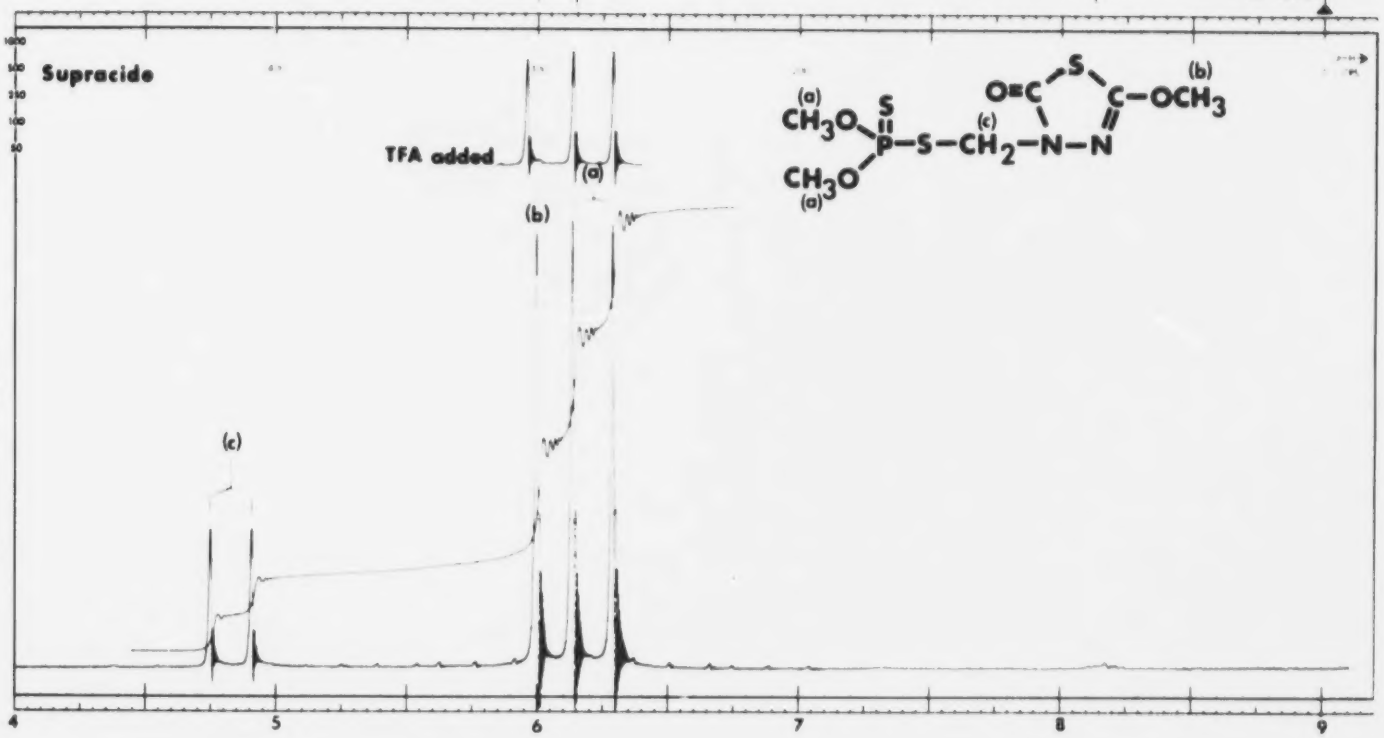
	T	J
a	8.82	7
b	8.72	7
c	8.1-8.9	
d	7.10	7
e	6.68	7
f	6.2	

C-33



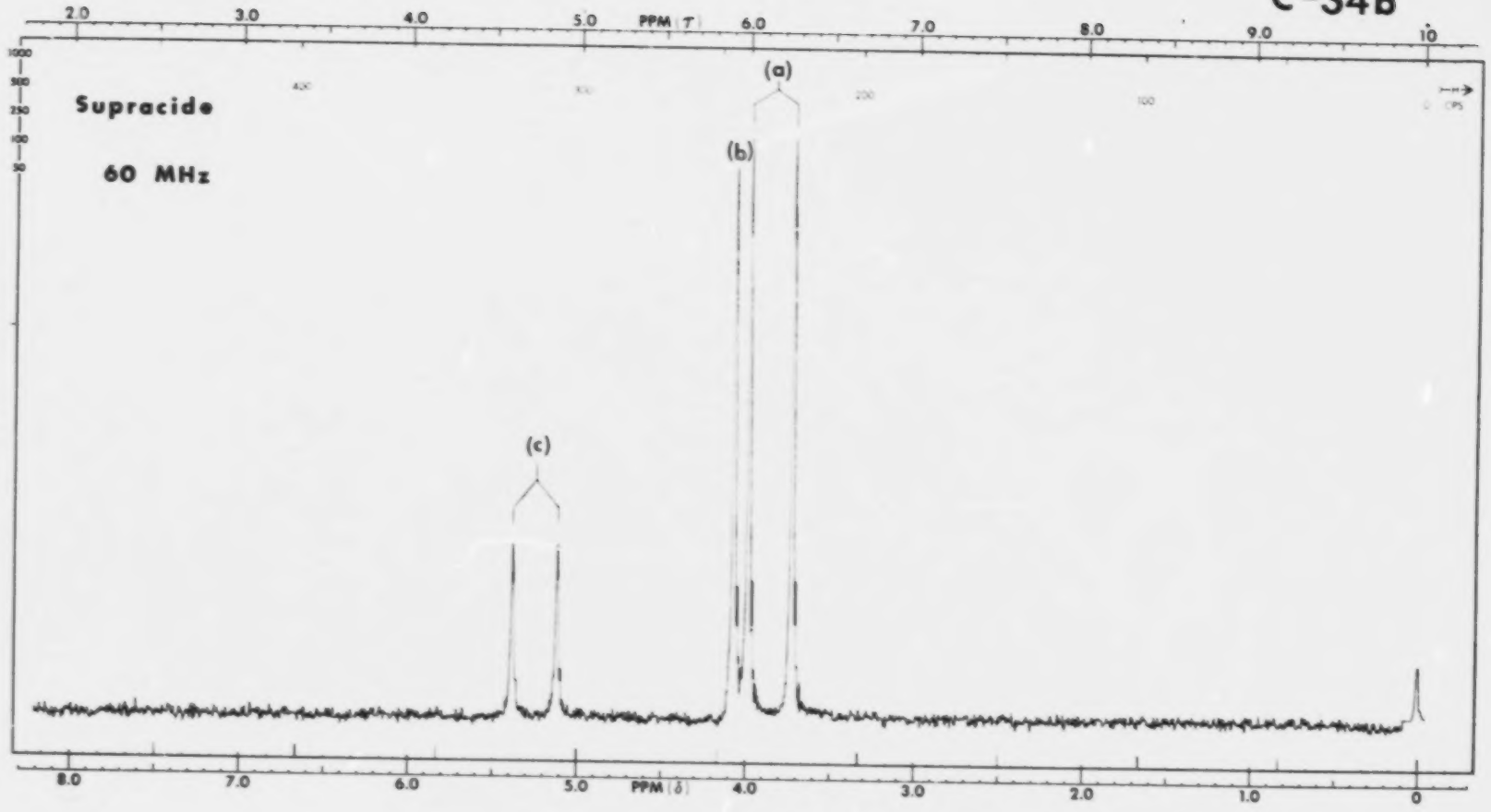
	T	J
a	8.72	7.5
b	8.2-8.5	
c	7.09	7.5
d	6.5	

C-34a

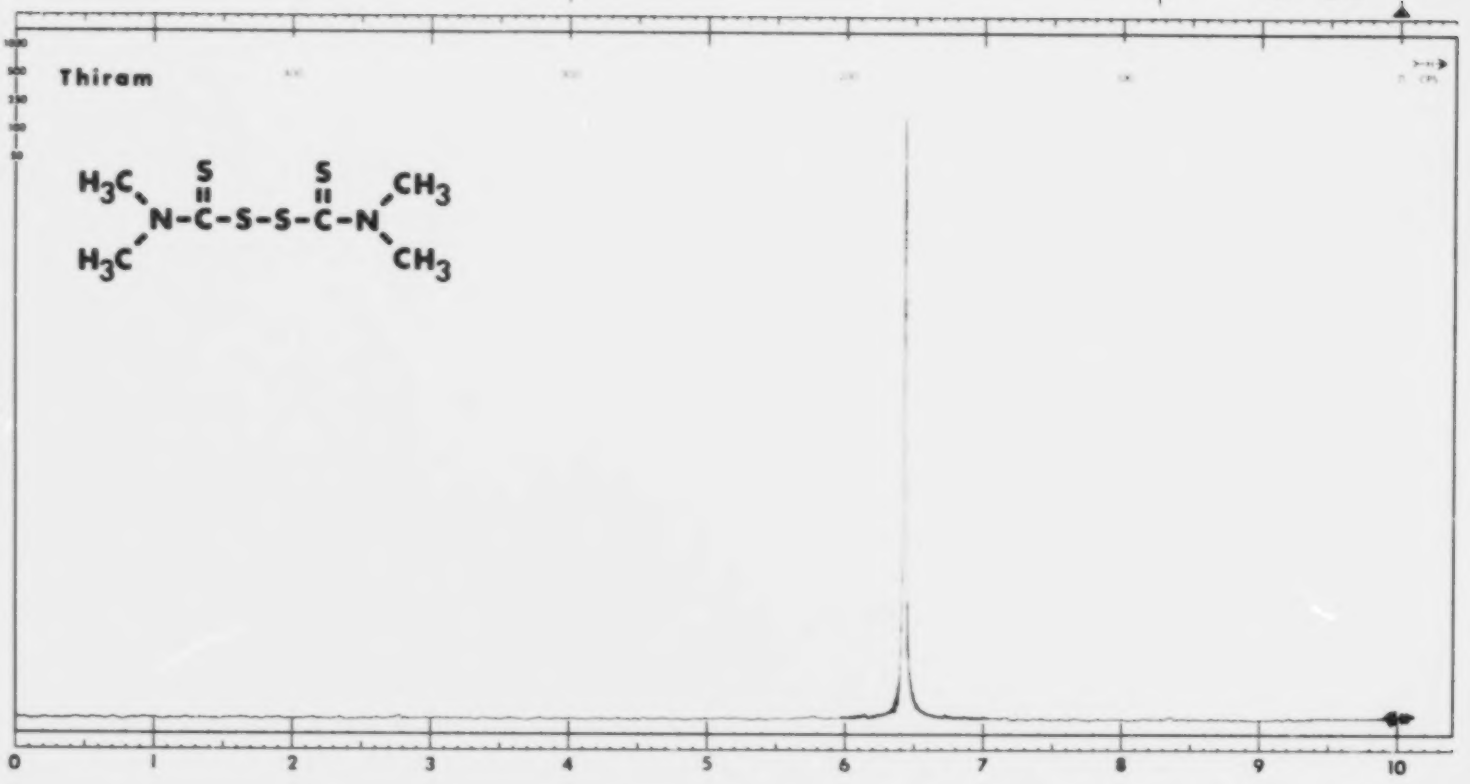


	τ	J
a	6.29	15
b	5.99	
c	4.82	16

C-34b

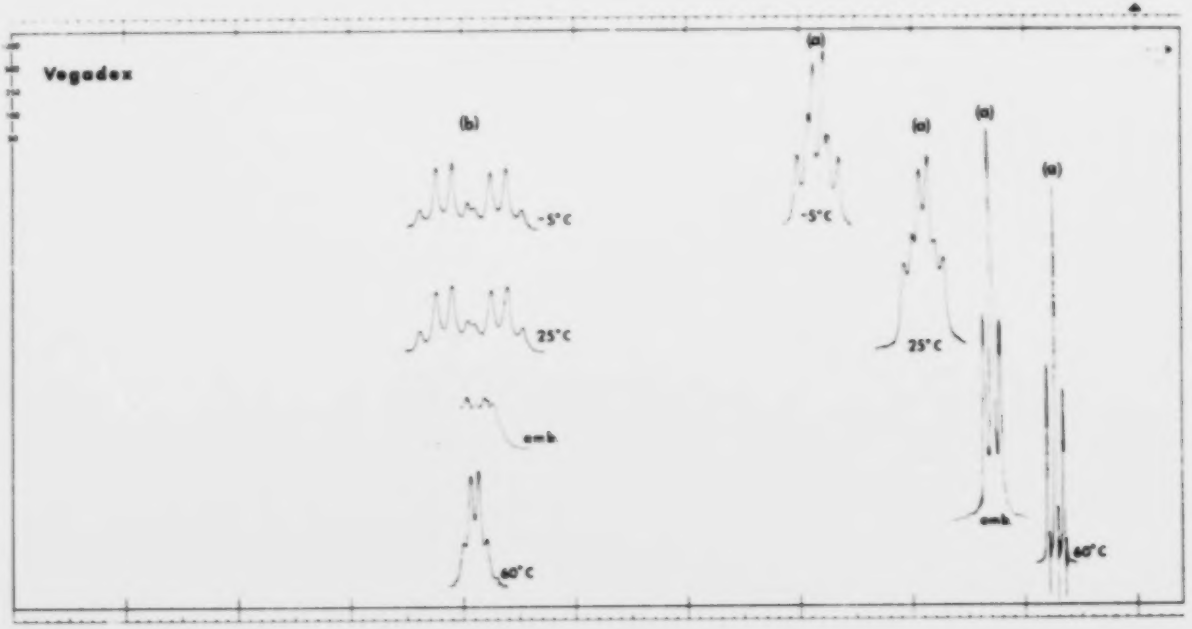

2.0
3.0
4.0
5.0
PPM (τ)
6.0
7.0
8.0
9.0
10
Supracide
60 MHz
(a)
(b)
(c)
8.0
7.0
6.0
5.0
PPM (δ)
4.0
3.0
2.0
1.0
0

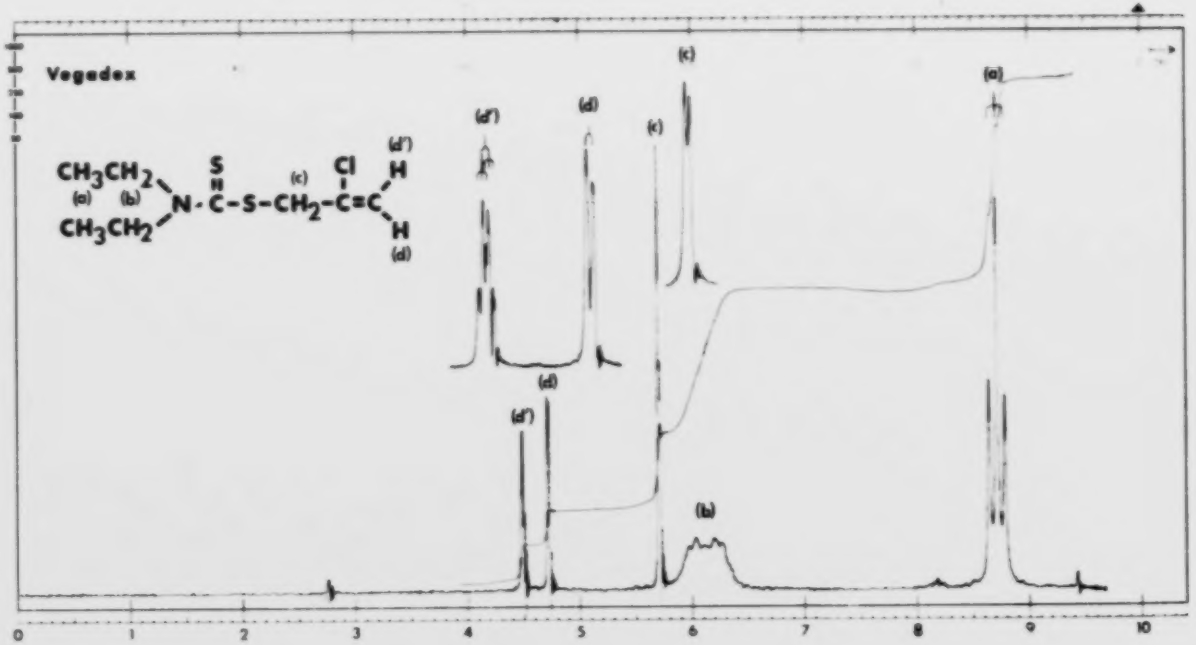
C-35



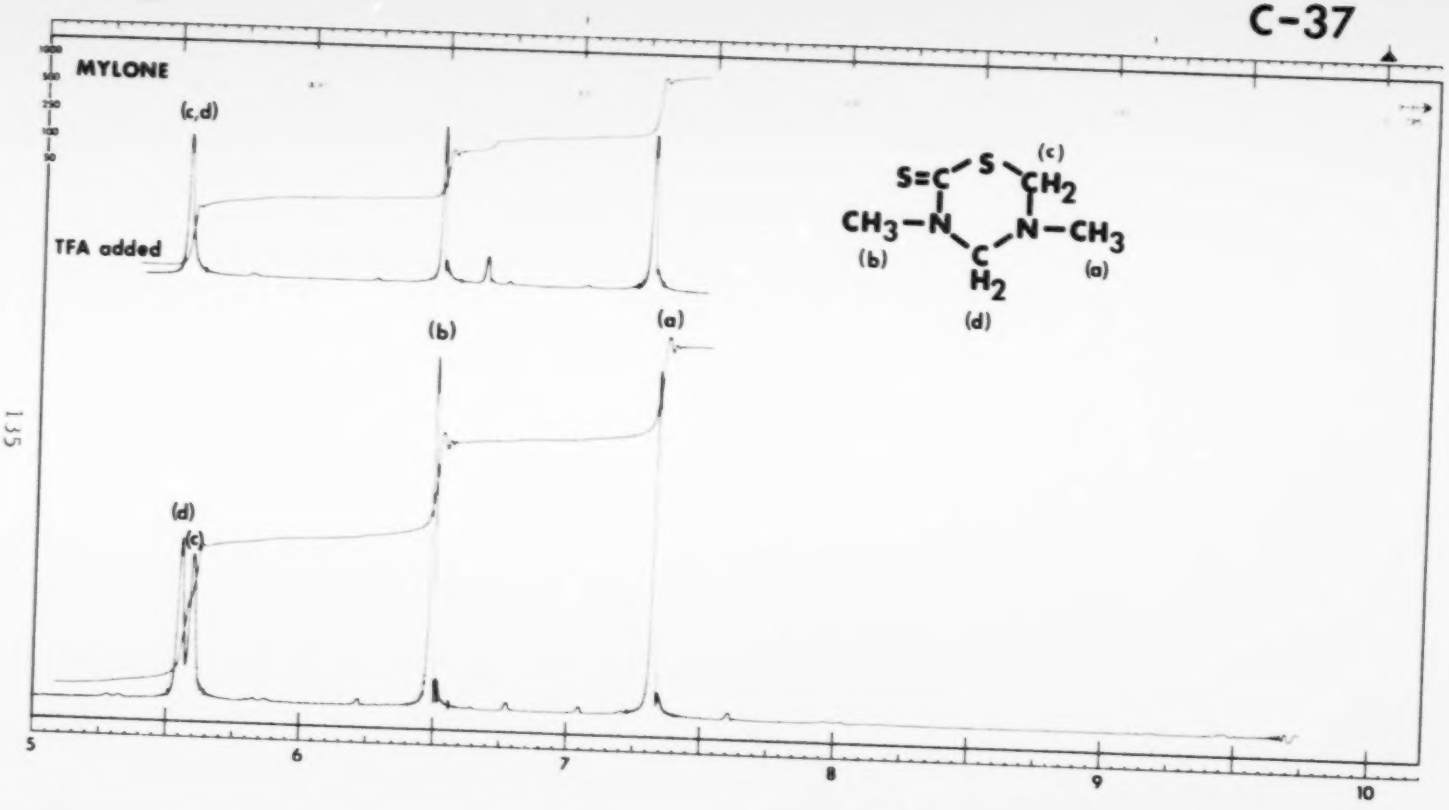
T

640





	T	J
a	8.72	7
b	6.12	7
c	5.72	$LO(H_c\text{-}H_d)$
d	4.73	$LS(H_d\text{-}H_d)$
d'	4.48	$LO(H_d\text{-}H_c)$ $LS(H_d\text{-}H_d)$



	T
a	7.28
b	6.49
c	5.59
d	5.55

SECTION IV

INDEX TO SPECTRA

Abate® - A-19

Acaralate - see Chloropropylate®

Alkron® - see Ethyl Parathion

Alleron® - see Ethyl Parathion

Aminocarb - see Matacil®

Anofex® - see p,p'-DDT

Aprocarb - see Baygon®

Arpocarb - see Matacil®

Aspon - A-46

Asuntol® - see Co-Ral®

Avadex® - C-30

Avadex BW - C-31

Azak - C-3

Azinphosethyl - see Ethyl Guthion®

Azinphosmethyl - see Guthion®

Azodrin® - A-10

Banol - see Carbanolate

Barban - C-24

Basudin® - see Diazinon

Baygon® - C-5

Baytex® - see Tiguvon

Benlate® - see Benomyl

Benomyl - C-7

Benomyl metabolite - C-8

Preceding page blank

Bidrin® - A-11

Bladafume - see Sulfotepp

Bulan® - B-22

Carbanolate - C-6

Carbaryl - see Sevin®

Carbicron - see Bidrin®

Carbofuran - see Furadan®

Carbophenothion - see Trithion®

Carbophos - see Malathion

Carbyne® - see Barban

CDEC - see Vegadex®

Chem-Hoe - see IPC

Chlorobenzilate - B-19

Chloro-IPC - see CIPC

Chloropham - See CIPC

Chloropropylate® - B-20

Ciodrin® - A-9

CIPC - C-23

Co-Ral® - A-40

Corothion - see Ethyl Parathion

Coumaphos - see Co-Ral®

Cygon® - A-3

Cygon oxygen analog - see Dimethoxon

Cynem - see Zinophos

Dalf® - see Methyl Parathion

DATC - see Avadex®

Dazomet - see Mylone

DBP - B-15

2,3 DCDT - see Avadex[R]

DDA - B-16

DDA Methyl Ester - B-17

o,p'-DDD - B-8

p,p'-DDD - B-7

DDE - B-11

DDMS - B-9

o,p'-DDMU - B-13

p,p'-DDMU - B-12

DDNU - B-14

DDOH - B-24

o,p'-DDT - B-2

p,p'-DDT - B-1

DDT acetal - B-26

DDT, Techical - B-3

DDVP - A-8

DEF[R] - A-49

Dedevap - see DDVP

DeGreen - see DEF[R]

Deleaf Defoliant - see Merphos

Delnav[R] - A-31

Demeton O - see Systox[R]

Demetron S - see Iso-Systox[R]

2,4-DEP - see Falone

Diallate - see Avadex[R]

Diazinon - A-37

Diazinon oxygen analog - see Diazoxon

Diazoxon - A-38

Dibrom[R] - A-6

Dicaptan[R] - see Dicapthon

Dicapthon - A-24

Dichlorophen (e) - see Preventol CD[R]

Dichlorvos - see DDVP

Dicofol - see Kelthane[R]

Dilan[R] - B-23

Dimecron[R] - see Phosphamidon

Dimethoate - see Cygon[R]

Dimethoxon - A-4

Dimethoxy DDT - see Methoxychlor

Dimetilan[R] - C-21

Dinocide[R] - see p,p'-DDT

Dioxathion - see Delnav[R]

Diphenamid - B-18

Dipteres - see Neguvon[R]

Dipterex - see Neguvon[R]

Disulfoton - see Di-Syston[R]

Di-Syston[R] - A-28

Dithiodemeton - see Di-Syston[R]

Dithione[R] - see Sulfotepp

Dithiosystox[R] - see Di-Syston

DMDT - see Methoxychlor

DMPA - see Zytron[R]

DMTT - see Mylone[R]

DNB - see Bulan[R]

DNP - see Prolan®

Dowco-139® - see Zectran®

Dow 1329® - see Zytron®

Dow ET-14® - see Ronnel (technical)

Dow ET-57® - see Ronnel (purified)

DTMC - see Kelthane®

Dursban® - A-35

Dupont Fungicide 1991 - see Benomyl

Dupont Fungicide 1991 metabolite - see Benomyl metabolite

Dylox® - see Neguvon

Dymid® - see Diphenamid

E-605 - see Ethyl Parathion

Easy Off-D - see Merphos

Enide - see Diphenamid

ENT 24, 969 - see Supona®

Entex® - see Tiguvon

EPN - A-44

EPN-300® - see EPN

Eptam® - C-26

EPTC - see Eptam®

Ethion - A-33

Ethyl Guthion® - A-39

Ethyl Parathion - A-41

Etilon - see Ethyl Parathion

Falodin - see Falone

Falone - A-47

Far-Go - see Avadex BW®

Fenchlorphos - see Ronnel

Fenthion - see Tiguvon

Folex® - see Merphos

Folidol® - see Ethyl Parathion

Folidol M - see Methyl Parathion

Folithion® - see Sumithion®

Forte - see Thiram

Fostion MM® - see Cygon®

Frumin AL® - see Di-Syston®

Frumin G® - see Di-Syston®

Furadan® - C-11

G-4® - see Preventol GD®

Gardentox - see Diazinon

Gardona® - A-21

Garrathion - see Trithion

GC-4072 - see Supona®

Genitox - see p,p'-DDT

Gesapon® - see p,p'-DDT

Gesarex® - see p,p'-DDT

Gesarol® - see p,p'-DDT

Guesapon® - see p,p'-DDT

Guesarol - see p,p'-DDT

Gusathion® - see Guthion

Gusathion A® - see Ethyl Guthion®

Guthion® - A-15

Guthion oxygen analog - A-16

Gyron® - see p,p'-DDT

Herkol - see DDVP

Hydram[R] - see Ordram[R]

Imidan[R] - A-17

INPC - see IPC

IPC - C-22

Isobutyl Triphenylmethylamine - B-27

Isolan - C-20

Isomeric Chlorthion[R] - see Dicapthon

Iso PPC - see IPC

Iso-Systox[R] - A-30

Ixodex[R] - see p,p'-DDT

Karbofos - see Malathion

Kelthane[R] - B-6

Korlan[R] - see Ronnel

Landrin - see SD-8530

Lannate[R] - see Methomyl

Lebaycid[R] - see Tiguvon

Mafu - see DDVP

Malaoxon - A-2

Malaspray - see Malathion

Malathion - A-1

Malathion oxygen analog - see Malaoxon

Malathon - see Malathion

Marlate - see Methoxychlor

Matacil[R] - C-13

MCA-600 - see Mobam

o-MDT - B-4

Mercaptophos - see Tiguvon

Mercapto dimethur - see Mesurol®

Merphos - A-48

Mesurol® - C-15

Metaisosystoxsulfoxide - see Meta-Systox-R®

Meta-Systox-R® - A-5

Methomyl - C-18

Methoxychlor - B-5

Methoxy DDT - see Methoxychlor

Methyl demeton-O-sulfoxide - see Meta-Systox-R®

Methyl Guthion® - see Guthion®

Methyl Parathion - A-22

Methyl Trithion - A-14

Metmercapturon - see Mesurol®

Metron - see Methyl Parathion

Mevinphos - see Phosdrin

Microfume - see Mylone®

Mintacol® - see Paraoxon

Mobam - C-12

Molinate - see Ordram®

Muscatox® - see Co-Ral®

Mylone® - C-37

Naled - see Dibrom®

Nankor® - see Ronnel

Navadel® - see Delnav

Neguvon® - A-7

Nemafos - see Zinophos

Nemaphos - see Zinophos

Neocid[R] - see p,p'-DDT

Neocidol - see p,p'-DDT

Niagara 1240[R] - see Ethion

Nialate[R] - see Ethion

Niran[R] - see Ethyl Parathion

Nitrostigmine - see Ethyl Parathion

Nitrox - see Methyl Parathion

Nitrox 80 - see Methyl Parathion

Nogos - see DDVP

Nomersan[R] - see Thiram

Nuvacren - see Azodrin[R]

Oko - see DDVP

Ordram[R] - C-33

Orthophos - see Ethyl Parathion

Oxydemetonmethyl - see Meta-Systox-R

Paraoxon - A-42

Parathion - see Ethyl Parathion

Parathion Methyl - see Methyl Parathion

Parathion oxygen analog - see Paraoxon

PEBC - see Tillam[R]

Pebulate - see Tillam[R]

Pentachlorin - see p,p'-DDT

Perfekthion - see Cygon

Perthane[R] - B-10

Phencapton - A-34

Phenkaptone[R] - see Phencapton

Phorate - see Thimet®

Phosdrin - A-12

Phosphamidon - A-13

Polyram-Ultra - see Thiram

Pomasol® - see Thiram

Preventol - see Preventol GD®

Preventol GD® - B-25

Preventol GDC® - see Preventol GD®

Primin - see Isolan

Prolan® - B-21

Prolate - see Imidan®

Propham - see IPC

Propoxur - see Baygon®

Queletox® - see Tiguvon

RE-5305 - C-4

Resitox - see Co-Ral

Rhodiatox® - see Ethyl Parathion

Rhothane® - p,p'-DDD

Rogor® - see Cygon®

Ro-Neet - C-32

Ronnel - A-20

Rowmate® - see Sirmate

Roxion - see Cygon

Ruelene® - A-25

S-847® - see Barban

SB-7859 - see Supona®

SD-8530 - C-1

Sevin® - C-9

Sirmate - mixture of 2,3-and 3,4-Sirmate

Sirmate,2,3,isomer - C-16

Sirmate,3,4 isomer - C-17

Sok - see Carbanolate

Solvirex® - see Di-Syston®

Spectracide - see Diazinon

Sulfatepp - see Sulfotepp

Sulfotepp - A-45

Sumithion® - A-23

Supona® - A-43

Supracide® - C-34

Sutan - C-27

Swep - C-25

Systox® - A-29

TDE - see p,p'-DDD

TEDTP - see Sulfotepp

Temik® - C-19

Terbutol - see Azak

Thimet® - A-27

Thiodemeton O - see Di-Syston®

Thiol-Systox - see Iso-Systox®

Thionazin - see Zinophos

Thiono-Systox - see Systox®

Thiophos® - see Ethyl Parathion

Thiotepp - see Sulfotepp

Thiram - C-35

Tiguvon - A-18

Tillam[R] - C-28

TMTD - see Thiram

TMTDS - see Thiram

Triallate - see Avadex BW

Trichlorofon - see Neguvon[R]

Trithion[R] - A-32

Trolene[R] - see Ronnel

Tuads - see Thiram

Tugon[R] - see Neguvon[R]

UC-8454 - C-10

UC-10854 - C-2

Unden[R] - see Baygon[R]

Vapona[R] - see DDVP

Vegadex[R] - C-36

Vernam[R] - C-29

Vernolate - See Vernam[R]

Viozene[R] - see Ronnel

Wepsin[R] - see Wepsyn[R]

Wepsyn[R] - A-50

Zectran[R] - C-14

Zinophos - A-36

Zytron[R] - A-26

SECTION V

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SECTION VIII

APPENDIX: CHEMICAL NAMES AND SOURCES OF THE PESTICIDES

Spectrum No.	Common or Trade Name	Chemical Name	Source
A-1	Malathion	O,O-Dimethyl S-(1,2-dicarboethoxyethyl) phosphorodithioate	American Cyanamid
A-2	Malaoxon	O,O-Dimethyl S-(1,2-dicarboethoxyethyl) phosphorothioate	American Cyanamid
A-3	Cygon®	O,O-Dimethyl S-(N-methylcarbamoylmethyl) phosphorodithioate	American Cyanamid
A-4	Dimethoxon	O,O-Dimethyl S-(N-methylcarbamoylmethyl) phosphorothioate	American Cyanamid
A-5	Meta-Systox-R®	O,O-Dimethyl S-[2-(ethylsulfinyl) ethyl] phosphorothioate	Chemagro Corp
A-6	Dibrom®	O,O-Dimethyl O-1,2-dibromo-2,2-dichloroethyl phosphate	Chevron Chem Co
A-7	Neguvon®	O,O-Dimethyl (1-hydroxy-2,2,2-trichloroethyl) phosphonate	Chemagro Corp
A-8	DDVP	O,O-Dimethyl O-2,2-dichlorovinyl phosphate	Shell Development Corp
A-9	Ciodrin®	α-Methylbenzyl 3-(dimethoxyphosphinyloxy)-cis-crotonate	Shell Development Corp
A-10	Azodrin®	3-(Dimethoxyphosphinyloxy)-N-methyl-cis-crotonamide	Shell Development Corp
A-11	Bidrin®	3-(Dimethoxylphosphinyloxy)-N,N-dimethyl-cis-crotonamide	Shell Development Corp

Spectrum No.	Common or Trade Name	Chemical Name	Source
A-12	Phosdrin®	O,O-Dimethyl O-(2-carbomethoxy-1-methylvinyl) phosphate	FDA
A-13	Phosphamidon	O,O-Dimethyl O-[2-chloro-2-(N,N-diethyl carbamoyl)-1-methylvinyl] phosphate	Chevron Chem Co
A-14	Methyl Trithion®	O,O-Dimethyl S-(p-chlorophenylthio)methyl phosphorodithioate	Stauffer Chem Co
A-15	Guthion®	O,O-Dimethyl S-[4-oxo-1,2,3-benzotriazin-3(4H)-yl methyl] phosphorodithioate	Chemagro Corp
A-16	Guthion oxygen analog	O,O-Dimethyl S-[4-oxo-1,2,3-benzotriazin-3(4H)-yl methyl] phosphorothioate	Chemagro Corp
A-17	Imidan®	O,O-Dimethyl S-phthalimidomethyl phosphorodithioate	Stauffer Chem Co
A-18	Tiguvon®	O,O-Dimethyl O-[4-(methylthio-m-tolyl] phosphorothioate	Chemagro Corp
A-19	Abate®	O,O,O',O'-Tetramethyl O,O'-thiodi-p-phenylene phosphorothioate	American Cyanamid
A-20	Ronnel	O,O-Dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate	Dow Chem Co
A-21	Gardona®	vinyl dimethyl ester 2-chloro-1-(2,4,5-trichlorophenyl) phosphoric acid	Shell Development Corp
A-22	Methyl parathion	O,O-Dimethyl O-(4-nitrophenyl) phosphorothioate	Monsanto Chem Co
A-23	Sumithion®	O,O-dimethyl O-(4-nitro-m-tolyl) phosphorothioate	Chemagro Corp

Spectrum No.	Common or Trade Name	Chemical Name	Source
A-24	Dicapthon	O,O-Dimethyl O-(2-chloro-4-nitrophenyl) phosphorothioate	American Cyanamid
A-25	Ruelene®	4-t-Butyl-2-chlorophenyl methyl methylphosphoramidate	Dow Chemical Co
A-26	Zytron®	2,4-Dichlorophenyl methyl isopropyl-phosphoramidothioate	Dow Chemical Co
A-27	Thimet®	O,O-Diethyl S-(ethylthio) methyl phosphorodithioate	American Cyanamid
A-28	Di-Syston®	O,O-Diethyl S-2-(ethylthio) ethyl phosphorodithioate	Chemagro Corporation
A-29	Systox®	O,O-Diethyl O-2-(ethylthio) ethyl phosphorothioate	Chemagro Corporation
A-30	Iso-Systox®	O,O-Diethyl S-2-(ethylthio) ethyl phosphorothioate	Chemagro Corporation
A-31	Delnav®	2,3-p-Dioxanedithiol S,S'-bis(O,O-diethyl phosphorodithioate)	Hercules Powder Company
A-32	Trithion®	O,O-Diethyl S-(4-chlorophenylthiomethyl) phosphorodithioate	Stauffer Chemical Co
A-33	Ethion	O,O,O',O'-Tetraethyl S,S'-methylene bis-phosphorodithioate	Niagara Chem Div, FMC Corp
A-34	Phenacapton	O,O-Diethyl S-(2,5-dichlorophenylthio) methyl phosphorodithioate	Geigy Chemical Corporation
A-35	Dursban®	O,O-Diethyl O-(3,5,6-trichloro-2-pyridyl) phosphorothioate	Dow Chemical Co

Spectrum No.	Common or Trade Name	Chemical Name	Source
A-36	Zinophos®	O,O-Diethyl O-2-pyrazinyl phosphorothioate	American Cyanamid
A-37	Diazinon	O,O-Diethyl O-(2-isopropyl-4-methyl-6-pyrimidyl) phosphorothioate	Geigy Chemical Corp
A-38	Diazoxon	O,O-Diethyl O-(2-isopropyl-4-methyl-6-pyrimidyl) phosphate	Geigy Chemical Corp
A-39	Ethyl Guthion®	O,O-Diethyl S- [4-oxo-1,2,3-benzotriazin-3-(4H)yl methyl] phosphorodithioate	Chemagro Corporation
A-40	Co-Ral®	O,O-Diethyl O-(3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl) phosphorothioate	Chemagro Corporation
A-41	Ethyl parathion	O,O-Diethyl O-4-nitrophenyl phosphorothioate	Monsanto Chemical Co
A-42	Paraoxon	O,O-Diethyl O-4-nitrophenyl phosphate	American Cyanamid
A-43	Supona®	O,O-Diethyl-1-(2,4-dichlorophenyl)-2-chlorovinyl phosphate	Shell Development Corp
A-44	EPN	O-Ethyl O-4-nitrophenyl phenylphosphonothioate	E. I. Dupont de Nemours and Co
A-45	Sulfotepp	O,O,O',O'-Tetraethyl dithiopyrophosphate	Chemagro Corporation
A-46	Aspon	O,O,O',O'-Tetrapropyl dithiopyrophosphate	Stauffer Chemical Co
A-47	Falone	Tris-(2,4-dichlorophenoxyethyl) phosphite	U S Rubber
A-48	Merphos	Tributyl phosphorotrithioite	V-C Chemical Co

Spectrum No.	Common or Trade Name	Chemical Name	Source
A-49	DEF[R]	S,S,S-Tributyl phosphorotrithioate	Chemagro Corporation
A-50	Wepsyn[R]	5-Amino-1-bis(diethylamido)phosphoryl-3-phenyl-1,2,4-triazole	Thompson-Hayward
B-1	p,p'-DDT	1,1,1-Trichloro-2,2-bis(p-chlorophenyl)-ethane	FDA
B-2	o,p'-DDT	1,1,1-Trichloro-2-p-chlorophenyl-2-o-chlorophenylethane	FDA
B-3	Tech DDT	Mixture of o,p'-DDT and p,p'-DDT	Allied Chemical Corp
B-4	o-MDT	1,1,1-Trichloro-2-o-chlorophenyl-2-phenylethane	CDC, PHS
B-5	Methoxychlor	1,1,1-Trichloro-2,2-bis (p-methoxyphenyl)-ethane	Geigy Chemical Corp
B-6	Kelthane[R]	1,1-bis(p-Chlorophenyl)-2,2,2-trichloro-ethanol	Rohm & Haas Co
B-7	p,p'-DDD	1,1-Dichloro-2,2-bis(p-chlorophenyl) ethane	FDA
B-8	o,p'-DDD	1,1-Dichloro-2-p-chlorophenyl-2-o-chlorophenylethane	FDA
B-9	DDMS	1-Chloro-2,2-bis(p-chlorophenyl) ethane	CDC, PHS
B-10	Perthane[R]	1,1-Dichloro-2,2-bis(p-ethylphenyl)-ethane	Rohm & Haas Co

Spectrum No.	Common or Trade Name	Chemical Name	Source
B-11	DDE	1,1-Dichloro-2,2-bis(p-chlorophenyl)-ethylene	FDA
B-12	p,p'-DDMU	1-Chloro-2,2-bis(p-chlorophenyl)ethylene	CDC, PHS
B-13	o,p'-DDMU	1-Chloro-2-p-chlorophenyl-2-o-chlorophenyl-ethylene	FDA
B-14	DDNU	1,1-bis(p-Chlorophenyl)ethylene	CDC, PHS
B-15	DBP	p,p'-Dichlorobenzophenone	Eastman Org Chem
B-16	DDA	bis(p-Chlorophenyl)acetic acid	CDC, PHS
B-17	DDA methyl ester	Methyl bis(p-chlorophenyl)acetate	CDC, PHS
B-18	Diphenamid	N,N-Dimethyl-2,2-diphenylacetamide	Upjohn Co
B-19	Chlorobenzilate	Ethyl-p,p'-dichlorobenzilate	Geigy Chemical Corp
B-20	Chloropropylate®	Isopropyl-p,p'-dichlorobenzilate	Geigy Chemical Corp
B-21	Prolan®	2-Nitro-1,1-bis(p-chlorophenyl)propane	Commercial Solvents Corp
B-22	Bulan®	2-Nitro-1,1-bis(p-chlorophenyl)butane	Commercial Solvents Corp
B-23	Dilan®	Mixture of Prolan and Bulan	Commercial Solvents Corp
B-24	DDOH	2,2-bis(p-Chlorophenyl)ethanol	CDC, PHS
B-25	Preventol® GD	bis(o-Hydroxy-p-chlorophenyl)methane	General Aniline & Film Corp
B-26	DDT acetal	2-bis(p-Chlorophenyl)methyl-1,3-dioxolane	CDC, PHS

Spectrum No.	Common or Trade Name	Chemical Name	Source
B-27	Isobutyl triphenyl-methylamine		Imperial Chem Industries LTD
C-1	SD 8530	3,4,5-Trimethylphenyl-N-methylcarbamate	Shell Development Corp
C-2	UC 10854	3-Isopropylphenyl-N-methylcarbamate	Union Carbide Corp
C-3	Azak®	2,6-Di-tert-butyl-4-methylphenyl-N-methylcarbamate	Hercules Powder Co
C-4	RE 5305	3-sec-Butylphenyl-N-methylcarbamate	Chevron Chemical Co
C-5	Baygon®	2-Isopropoxyphenyl-N-methylcarbamate	Chemagro Corporation
C-6	Carbanolate	3,4-Xylyl-6-chloro-N-methylcarbamate	Upjohn Company
C-7	Benomyl	Methyl 1-(butylcarbamoyl)-2-benzimidazole carbamate	E. I. DuPont de Nemours & Co
C-8	Benomyl metabolite	Methyl 5-hydroxy-2-benzimidazole carbamate	E. I. DuPont de Nemours & Co
C-9	Sevin®	1-Naphthyl-N-methylcarbamate	Union Carbide Corporation
C-10	UC 8454	1-(5,6,7,8-Tetrahydro)-naphthyl-N-methylcarbamate	Union Carbide Corporation
C-11	Furadan®	7-(2,3-Dihydro-2,2-dimethyl)-benzofuranyl-N-methylcarbamate	Niagara Chemical Div, FMC Corp
C-12	Mobam®	4-Benzothienyl-N-methylcarbamate	Mobil Chemical Co
C-13	Matacil®	4-Dimethylamino-3-methylphenyl-N-methylcarbamate	Chemagro Corporation

Spectrum No.	Common or Trade Name	Chemical Name	Source
C-14	Zectran[R]	4-Dimethylamino-3,5-dimethylphenyl-N-methylcarbamate	Dow Chemical Co
C-15	Mesurol[R]	4-Methylthio-3,5-dimethylphenyl-N-methylcarbamate	Chemagro Corporation
C-16	Sirmate, 2,3-isomer	2,3-Dichlorobenzyl-N-methylcarbamate	FDA
C-17	Sirmate, 3,4-isomer	3,4-Dichlorobenzyl-N-methylcarbamate	FDA
C-18	Methomyl	S-Methyl N-[(methylcarbamoyl)oxy] thioacetimidate	E. I. DuPont de Nemours & Co
C-19	Temik[R]	2-Methyl-2-methylthiopropionaldehyde-O-methylcarbamoyl oxime	Union Carbide Corp
C-20	Isolan	5-(1-Isopropyl-3-methyl)-pyrazolyl-N,N-dimethylcarbamate	Geigy Chemical Corp
C-21	Dimetilan[R]	3-(1-N,N-Dimethylcarbamoyl-5-methyl)-pyrazolyl-N,N-dimethylcarbamate	Geigy Chemical Corp
C-22	IPC	Isopropyl-N-phenylcarbamate	Pittsburgh Plate Glass Co
C-23	CIPC	Isopropyl-N-(3-chlorophenyl)carbamate	Pittsburgh Plate Glass Co
C-24	Barban	4-Chloro-2-butynyl-N-(3-chlorophenyl)-carbamate	Gulf Res & Dev Co
C-25	Swep	Methyl-N-(3,4-dichlorophenyl)carbamate	Niagara Chem Div, FMC Corp
C-26	Eptam[R]	S-Ethyl-N,N-dipropylthiolcarbamate	Stauffer Chemical Co
C-27	Sutan	S-Ethyl-N,N-diisobutylthiolcarbamate	Stauffer Chemical Co

Spectrum No.	Common or Trade Name	Chemical Name	Source
C-28	Tillam[R]	S-Propyl-N-butyl-N-ethylthiolcarbamate	Stauffer Chemical Co
C-29	Vernam[R]	S-Propyl-N,N-dipropylthiolcarbamate	Stauffer Chemical Co
C-30	Avadex[R]	S-(2,3-Dichloroallyl)-N,N-diisopropyl thiolcarbamate	Monsanto Chemical Co
C-31	Avadex BW[R]	S-(2,3,3-Trichloroallyl)-N,N-diisopropyl thiolcarbamate	Monsanto Chemical Co
C-32	Ro-Neet	S-Ethyl-N-ethyl-N-cyclohexylthiolcarbamate	Stauffer Chemical Co
C-33	Ordram[R]	S-Ethyl-hexahydroazepine-1-carbothioate	Stauffer Chemical Co
C-34	Supracide[R]	O,O-Dimethyl-S-[2-methoxy-1,3,4-thiadiazol-5(4H)-onyl-4-methyl]-dithiophosphate	Geigy Chemical Corp
C-35	Thiram	bis(Dimethylthiocarbamoyl)disulfide	E. I. DuPont de Nemours & Co
C-36	Vegadex[R]	2-Chloroallyl-N,N-diethyl dithiocarbamate	Monsanto Chemical Co
C-37	Mylone[R]	3,5-Dimethyl-1,3,5-tetrahydrothiadiazine-2-thione	Union Carbide Corp

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27 Abstract

This catalog contains the 100 MHz nuclear magnetic resonance spectra of 114 organophosphorus, DDT, and carbamate pesticides and a brief discussion of their most important features. Chemical shifts and coupling constants are shown on each spectrum. (Alford - Southeast Water Laboratory)

Abstractor ANN L. ALFORD | Institution SOUTHEAST WATER LABORATORY

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